Quantum Simulation of the Agassi Model in Trapped Ions: determining the shape of the system

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Quantum Computing for Many-Body problems (QCMB): atomic nuclei, neutrinos, and other strongly correlated Fermi systems

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Outline

Why the Agassi model?

- 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.
- Nowadays, it is used to benchmark many-body approximations because of its great flexibility and simplicity to be solved for large systems.
- The model (and in particular its extension) 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.

What a (digital) Quantum Computer is?

A device composed of:

- m **2-level** quantum systems (qubits),
- a set of quantum gates (acting as unitary operators),
- a set of measurement operators (measuring the state of defined subset of qubits),
- a classical control unit which determines which gate should be applied.

I. M. Georgescu, S. Ashhab, and Franco Nori, Rev. Mod. Phys. **86**, 153 (2014).

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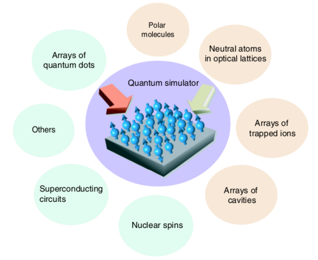
Implementations

- Trapped ions.
- Superconducting cirquits.
- Nuclear spins (NMR).
- Photons.
- Neutral atoms.
- Cavity arrays.



Outline

Agassi model

The first appearance

"Validity of the BCS and RPA approximations in the pairing-plus-monopole solvable model", Dan Agassi, Nuclear Physics A **116**, 49 (1968).

The original Hamiltonian

$$
\begin{aligned}
H &= \frac{1}{2}\epsilon \sum_{m\sigma} \sigma a^{\dagger}_{m\sigma} a_{m\sigma} + \frac{1}{2} V \sum_{mm'\sigma} a^{\dagger}_{m\sigma} a^{\dagger}_{m'\sigma} a_{m'-\sigma} a_{m-\sigma} \\
&\quad - \frac{1}{4} g \sum_{mm'\sigma\sigma'} a^{\dagger}_{m\sigma} a^{\dagger}_{-m\sigma} a_{-m'-\sigma'} a_{m'\sigma'}
\end{aligned}
$$

$\sigma = +1, -1$ and $m = -j, \ldots, -2, -1, 1, 2, \ldots, j$. Degeneracy $\Omega = 2j$

Agassi model

The O(5) as the spectrum generator algebra

$$J^+ = \sum_{m=-j}^{j} c^\dagger_{1m} c_{-1m} = \left(J^-\right)^\dagger ; \quad J^0 = \frac{1}{2} \sum_{m=-j}^{j} \left(c^\dagger_{1m} c_{1m} - c^\dagger_{-1m} c_{-1m}\right)$$

$$A^\dagger_1 = \sum_{m=1}^{j} c^\dagger_{1m} c^\dagger_{1,-m}; \quad A^\dagger_{-1} = \sum_{m=1}^{j} c^\dagger_{-1m} c^\dagger_{-1,-m}; \quad A^\dagger_0 = \sum_{m=1}^{j} \left(c^\dagger_{-1m} c^\dagger_{1,-m} - c^\dagger_{-1-m} c^\dagger_{1,m}\right)$$

$$N_\sigma = \sum_{m=-j}^{j} c^\dagger_{\sigma m} c_{\sigma m}, \qquad N = N_1 + N_{-1}$$

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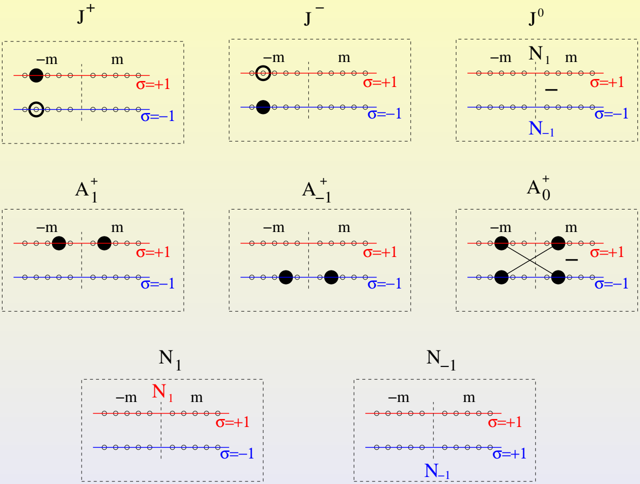
The Hamiltonian

$$H = \varepsilon J^0 - g \sum_{\sigma\sigma'} A^\dagger_\sigma A_{\sigma'} - \frac{V}{2}\left[\left(J^+\right)^2 + \left(J^-\right)^2\right] - 2hA^\dagger_0 A_0$$

For convenience

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

A pictorial view



Outline

The phases of the system

- The spherical phase: $\varphi = 0$ and $\beta = 0$.
- The Hartree-Fock deformed phase: $\varphi \neq 0$ and $\beta = 0$.
- The BCS deformed phase: $\varphi = 0$ and $\beta \neq 0$.
- The Hartree-Fock plus BCS deformed phase: $\varphi \neq 0$ and $\beta \neq 0$.

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In the original formulation of the Agassi model only the three first phases were present, but in the extended version of the model the four basis can be found and, moreover, there is coexistence of some of the phases.

The energy surfaces

φ Hartree-Fock variational parameter. β Bogoliubov variational parameter

The energy surface A

$$E_A = -\varepsilon j \cos\varphi \cos\beta - g j^2 \sin^2\beta - V j^2 \sin^2\varphi \cos^2\beta$$

$$\frac{E_A}{j\varepsilon} = -\cos\varphi\cos\beta - \frac{\Sigma}{2}\sin^2\beta - \frac{\chi}{2}\sin^2\varphi\cos^2\beta$$

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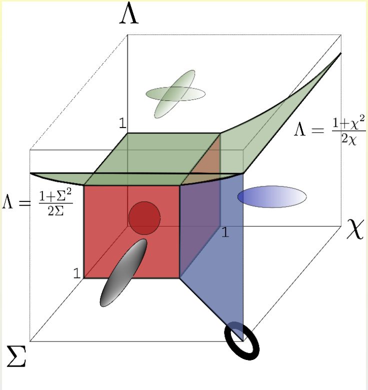
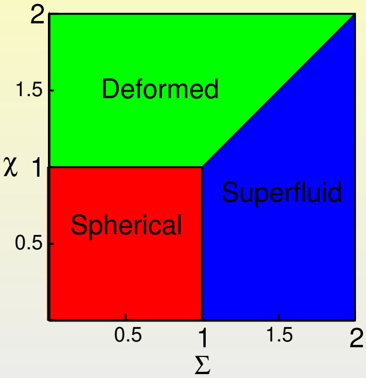
The energy surface B

$$E_B = -\varepsilon j \cos\varphi \cos\beta - 2h j^2 \sin^2\beta \sin^2\varphi - V j^2 \sin^2\varphi \cos^2\beta$$

$$\frac{E_B}{j\varepsilon} = -\cos\varphi\cos\beta - \Lambda\sin^2\beta\sin^2\varphi - \frac{\chi}{2}\sin^2\varphi\cos^2\beta$$

The phase diagram





Phase transition for the extended and simple Agassi model

(JEGR, J. Dukelsky, P. Pérez-Fernández, and J. M. Arias, PRC **97**, 054303 (2018))

Numerical calculations

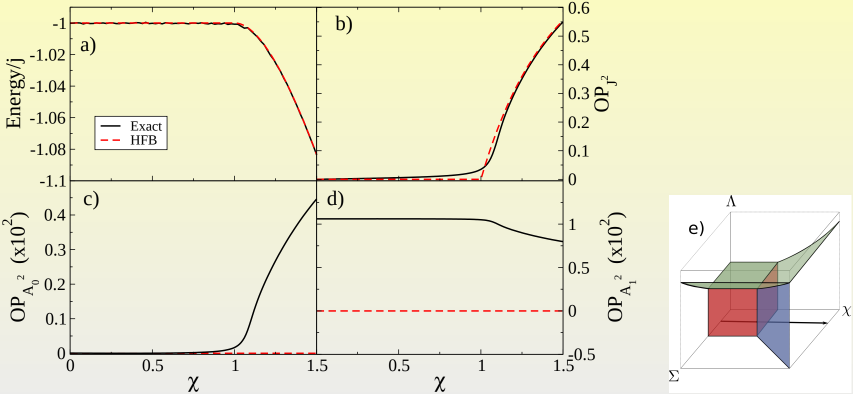


Figure: Comparison of HFB and exact results. $j = 100$ and Hamiltonian parameters $\Sigma = 0.5$, $\Lambda = 0$.

Numerical calculations

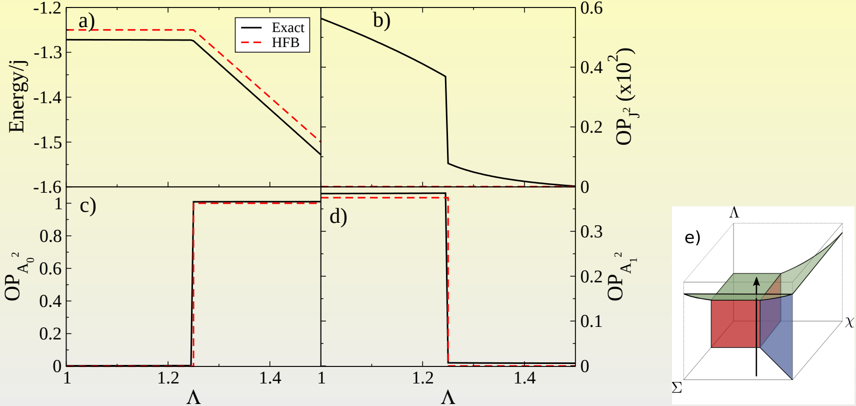


Figure: Comparison of HFB and exact results. $j = 100$ and Hamiltonian parameters $\chi = 1.5$, $\Sigma = 2$.

Outline

The Jordan-Wigner transformation

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

The transformation

$$c_i^\dagger = I_1 \otimes \ldots \otimes I_{i-1} \otimes \sigma_i^+ \otimes \sigma_{i+1}^z \otimes \ldots \otimes \sigma_N^z \,,$$
$$c_i = I_1 \otimes \ldots \otimes I_{i-1} \otimes \sigma_i^- \otimes \sigma_{i+1}^z \otimes \ldots \otimes \sigma_N^z \,,$$

with

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

and

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

The case of 4 sites, $j = 1$

The mapping of the building blocks

$$
\begin{aligned}
c_{1,1} &\rightarrow c_1, \\
c_{1,-1} &\rightarrow c_2, \\
c_{-1,1} &\rightarrow c_3, \\
c_{-1,-1} &\rightarrow c_4.
\end{aligned}
$$

$$
\begin{aligned}
J^+ &= -\sigma_2^+ \otimes \sigma_3^z \otimes \sigma_4^- - \sigma_1^+ \otimes \sigma_2^z \otimes \sigma_3^-, \\
J^0 &= (1/4)(\sigma_1^z + \sigma_2^z - \sigma_3^z - \sigma_4^z), \\
J^- = (J^+)^\dagger &= -\sigma_2^- \otimes \sigma_3^z \otimes \sigma_4^+ - \sigma_1^- \otimes \sigma_2^z \otimes \sigma_3^+, \\
A_1^\dagger &= \sigma_1^+ \otimes \sigma_2^+, \; A_{-1}^\dagger = \sigma_3^+ \otimes \sigma_4^+, \\
A_1 &= \sigma_1^- \otimes \sigma_2^-, \; A_{-1} = \sigma_3^- \otimes \sigma_4^-.
\end{aligned}
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The case of 4 sites, $j = 1$

The mapping of the building blocks

$$\begin{aligned} c_{1,1} &\to c_1, \\ c_{1,-1} &\to c_2, \\ c_{-1,1} &\to c_3, \\ c_{-1,-1} &\to c_4. \end{aligned}$$

$$\begin{aligned} J^+ &= -\sigma_2^+ \otimes \sigma_3^z \otimes \sigma_4^- - \sigma_1^+ \otimes \sigma_2^z \otimes \sigma_3^-, \\ J^0 &= (1/4)(\sigma_1^z + \sigma_2^z - \sigma_3^z - \sigma_4^z), \\ J^- = (J^+)^\dagger &= -\sigma_2^- \otimes \sigma_3^z \otimes \sigma_4^+ - \sigma_1^- \otimes \sigma_2^z \otimes \sigma_3^+, \\ A_1^\dagger &= \sigma_1^+ \otimes \sigma_2^+, \; A_{-1}^\dagger = \sigma_3^+ \otimes \sigma_4^+, \\ A_1 &= \sigma_1^- \otimes \sigma_2^-, \; A_{-1} = \sigma_3^- \otimes \sigma_4^-. \end{aligned}$$

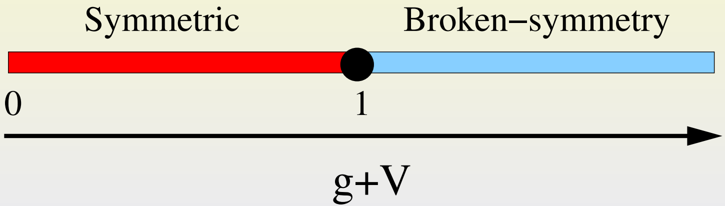
The Hamiltonian

$$\begin{aligned} H &= H_1 + H_2 + H_3, \\ H_1 &= \frac{\epsilon - g}{4}(\sigma_1^z + \sigma_2^z) - \frac{\epsilon + g}{4}(\sigma_3^z + \sigma_4^z), \\ H_2 &= -\frac{g}{4}(\sigma_1^z \otimes \sigma_2^z + \sigma_3^z \otimes \sigma_4^z), \\ H_3 &= -(g + V)(\sigma_1^+ \otimes \sigma_2^+ \otimes \sigma_3^- \otimes \sigma_4^- + \sigma_1^- \otimes \sigma_2^- \otimes \sigma_3^+ \otimes \sigma_4^+). \end{aligned}$$

$$[H_1, H_2] = 0, \qquad [H_2, H_3] = 0, \qquad [H_1, H_3] \neq 0.$$

The phase diagram (1D) for 4 sites, $j = 1$

- For $j = 1 \Rightarrow N = 4$ sites: $g = \Sigma$ and $V = \chi$
- The hamiltonian only depends on $g + V$
- Two phases: symmetric $g + V < 1$ and broken symmetry $g + V > 1$



Outline

What do we measure?

The evolution operator

$$U(t) = \exp(-i\ H\ t)$$

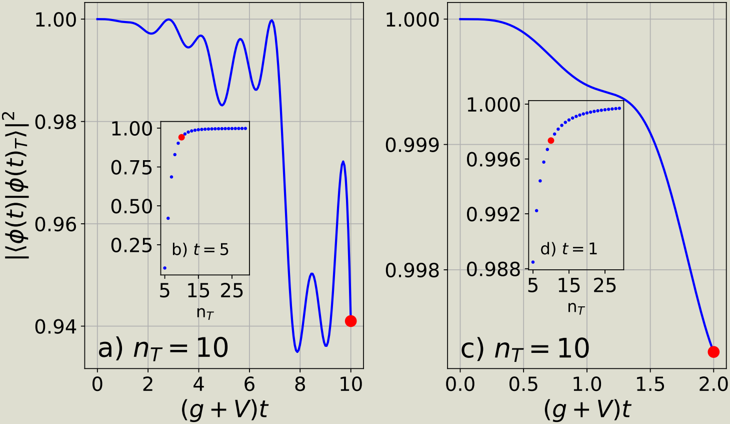
Experimentally it is implemented through the Lie-Trotter-Suzuki decomposition (Trotter in short)

$$U(t) \simeq \{\exp[-i(H_1 + H_2)(t/n_T)] \exp[-iH_3(t/n_T)]\}^{n_T},$$

where the error produced will depend on the commutator $[(H_1 + H_2), H_3]$ and scale as $1/n_T$, where n_T denotes the number of Trotter steps.

How good is the Trotter approach?

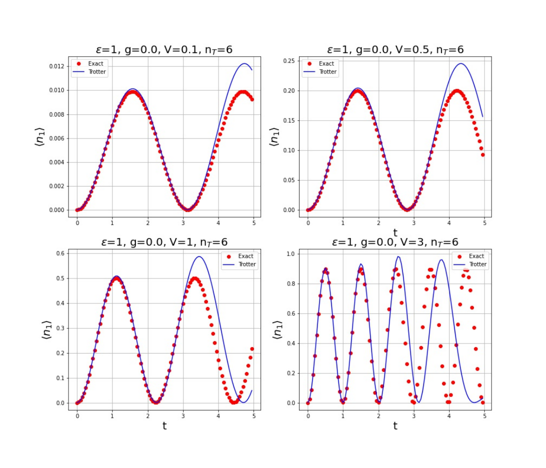
The fidelity



The initial state is $|\downarrow_1 \otimes \downarrow_2 \otimes \uparrow_3 \otimes \uparrow_4\rangle$ (with minimum value of $\langle J^0 \rangle = -1$). The parameters of the Hamiltonian are $\epsilon = 1$ and $g = V = 1$.

How good is the Trotter approach?

The value of $\langle n_1 \rangle$



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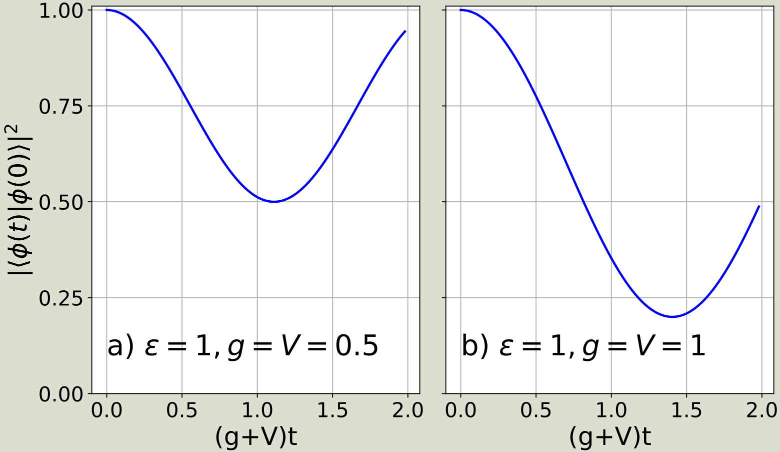
The survival probability



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Feasibility

- $\exp(-iH_1 t)$: single-qubit gates with fidelities often above 99.99% (in trapped ions).
- $\exp(-iH_2 t)$: two two-qubit gates carried out via Mølmer-Sørensen gates with fidelities above 99.9%, plus single-qubit gates to rotate the basis from x to z.
- $\exp(-iH_3 t)$: two Mølmer-Sørensen gates and a local gate, plus single qubit gates to rotate the bases. All the terms of H_3 are implemented with a single Trotter step.

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- The scaling of our protocol is efficient: the number of elementary gates is polynomial in the number of interacting fermions, N.
- With a classical computer the scaling would be inefficient*: the Hilbert space dimension would grow exponentially in N.
- 4-qubit proposal: 52 single-qubit gates and 50 two-qubits gates. Assuming gate errors of 0.0001 for the single-qubit and 0.001 for the two-qubit one, the total gate error, assuming $n_T = 5$, with be $E_G \simeq 0.28$ (fidelity above 70%).

Outline

Is it possible to determine the shape/phase of the system?

The obvious things

- Shape is not really an observable.
- The shape of the system is a property of its ground state (it is true that it can be also defined for a excited state).
- It is well defined at the mean-field level.

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A different view

- The shape of the system characterizes its spectrum.

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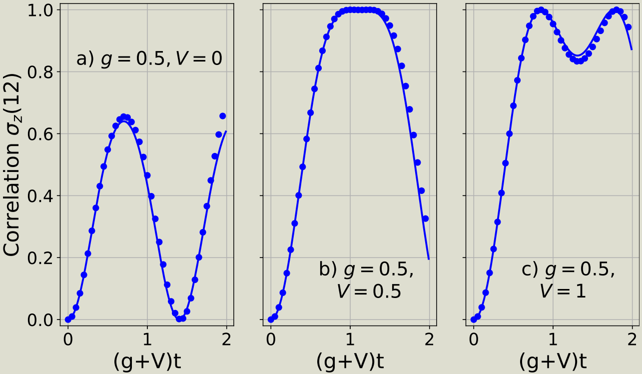
A different view

- The shape of the system characterizes its spectrum.
- An observable depending on the spectrum could encode the shape of the system. That, in general, will happen for the time evolution of the matrix element of a non-eigenstate.
- Most probably the results will depend on the state and on the used operator. Difficult to determine a priori the best state and operator.
- These types of measurements are the easiest ones in Quantum Computing.

Is it possible to determine the phase of the system?

The correlation function

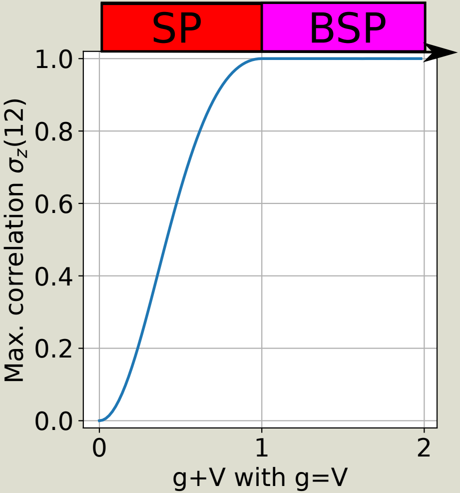
$$\sigma_z(1,2) \equiv \langle \sigma_1^z \sigma_2^z \rangle - \langle \sigma_1^z \rangle \langle \sigma_2^z \rangle$$



The initial state is $| \downarrow_1 \otimes \downarrow_2 \otimes \uparrow_3 \otimes \uparrow_4 \rangle$ (exact and Trotter results).

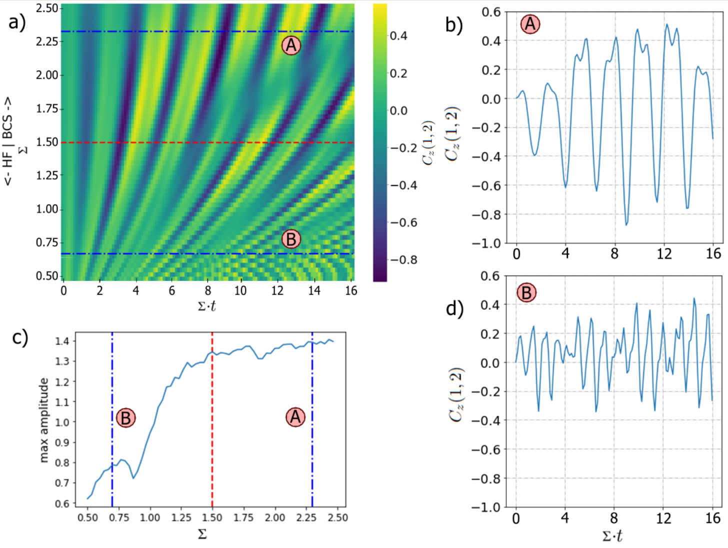
Is it possible to determine the phase of the system?

The maximum value of the correlation function as an "order parameter"



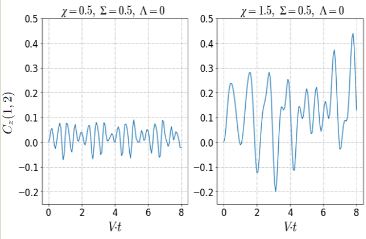
Outline

How to determine the phase in this case?

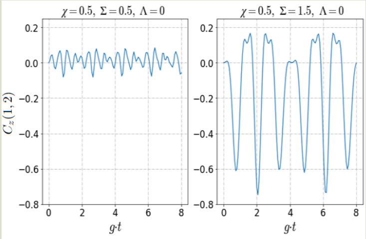


Different patterns everywhere

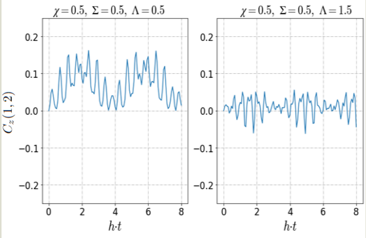
Symmetric HF



Symmetric BCS



Symmetric Combined



A different approach: machine learning to recognize the shape of the system

Machine learning in a classical computer

- Regression
- Clustering
- Decision Trees
- Reinforced Learning
- Genetic Algorithms
- **Neural Networks**

The recipe

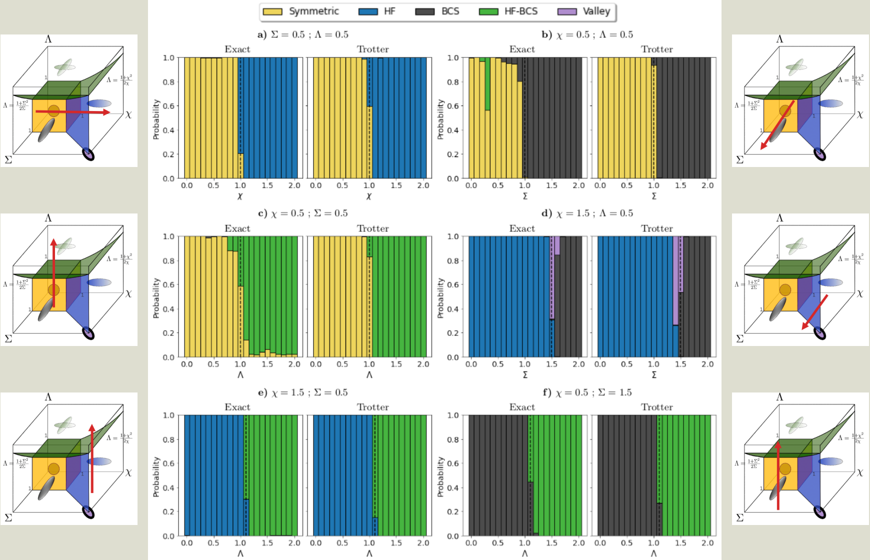
- To use supervised learning.
- Consider the knowledge of the phase diagram to define the categories.
- Train the algorithm with the time evolution of the correlation function.

Steps to implement a Convolutional Neural Network

Machine learning in a classical computer

- **Convolution layer**: the layer responsible of performing the convolution operation.
- **Activation layer**: the layer that applies the activation function together with the filter of the convolution layer.
- **Pooling layer**: the pooling layer performs a dimension reduction of the data, collapsing data by connecting clusters of neurons to a single neuron each.
- **Dropout layer**: this optional layer temporarily deactivates, or *drops out*, randomly selected training parameters from the previous layer that has trainable parameters. Its goal is to avoid the "overfitting".
- **Fully Connected layer**: Also know as *dense* layers, they connect every neuron of the input to every neuron of the output.
- **Softmax layer**: This layer is a fully connected or dense layer that applies a specific kind of activation function, called a *softmax* function, which is a normalized exponential function.

Results for a Convolutional Neural Network



Outline

Conclusions and outlook

- It has been proposed and analyzed the quantum simulation of the Agassi model for a size $N = 4$.
- Numerical simulations and analytical estimations show that this protocol is feasible with current technology.
- Time dynamics of a quantum correlation function allows to determine the different quantum phases of the model.
- The analysis has been extended up to $N = 8$ and to the full fledged Agassi model.
- Machine learning has shown its power to recognize phases in cases where noise is present.

Further reading

- P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata, "A digital quantum simulation of the Agassi model", Physics Letters B **829**, 137133 (2022).
- A. Sáiz, J.E. García-Ramos, J.M. Arias, L. Lamata, and P. Pérez-Fernández, "A digital quantum simulation of an extended Agassi model: using machine learning to disentangle its phase-diagram", arXiv:2205.15122.

Thank you for your attention