What Quantum Computing can do for Nuclear Physics?

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FÍSICA MATEMÁTICAS COMPUTACIÓN

Universidad de Huelva

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Overview

- What is Quantum Computing?
  - Bits and Qubits. Gates and quantum gates
- First applications in Nuclear Physics
- Other selected applications
  - Shell model calculations
  - The phase diagram of the Agassi model
- Conclusions

What is Quantum Computing?

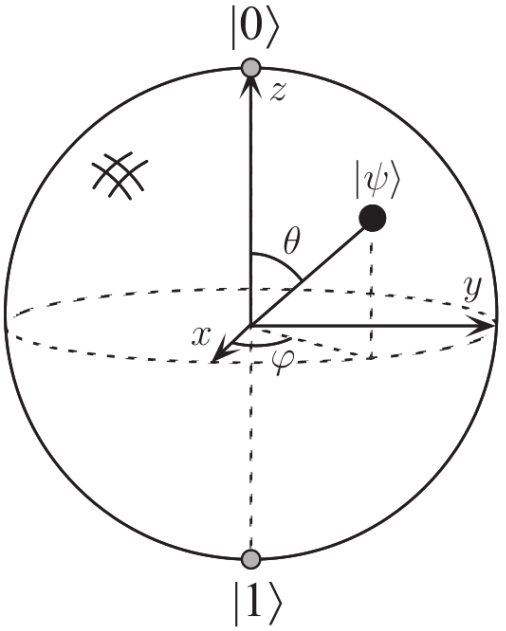
Bits and qubits

Bits: 0 or 1

Qubits:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$



Bloch sphere

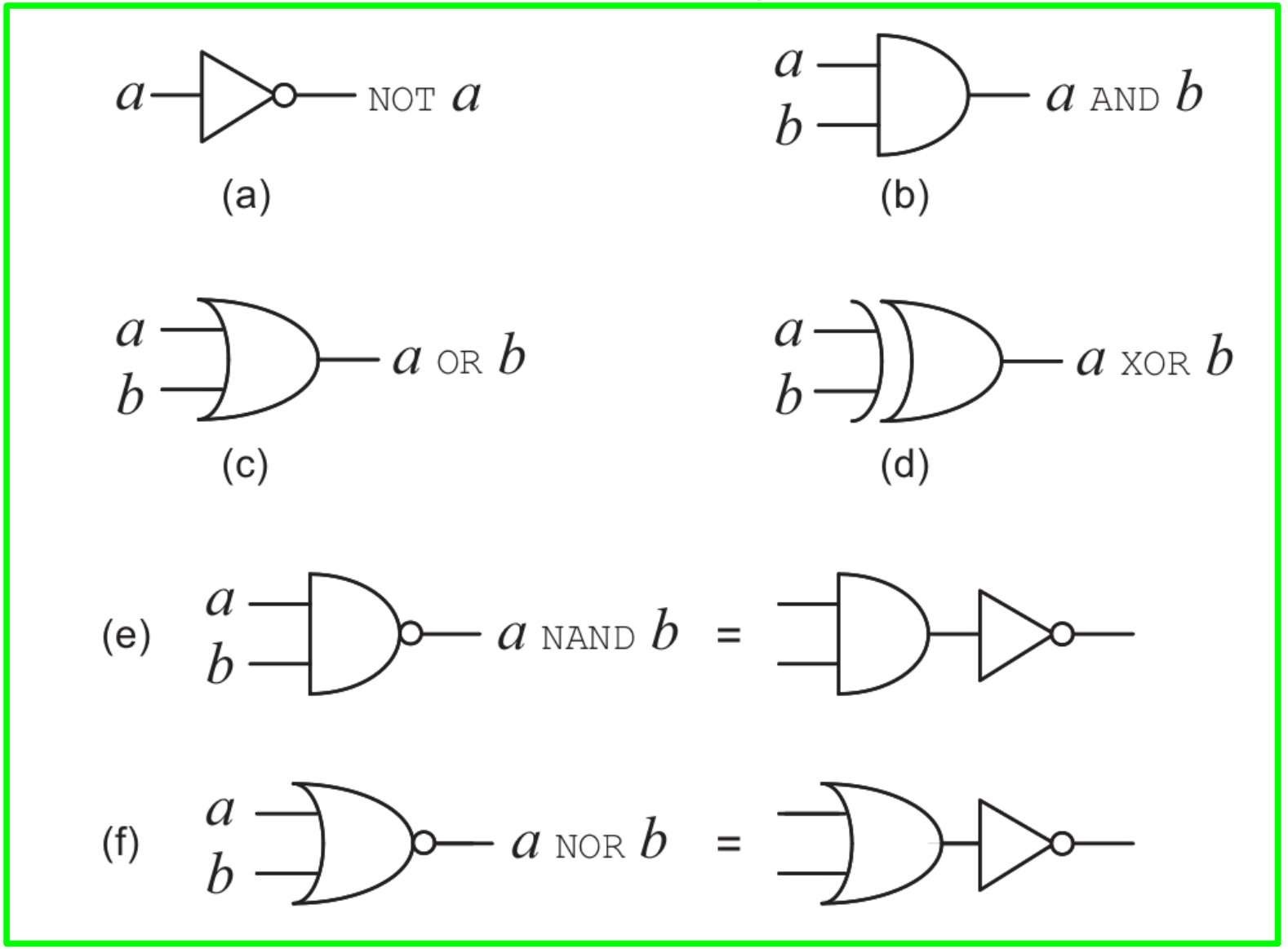
Multiple Qubits:

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Bell state: $\dfrac{|00\rangle + |11\rangle}{\sqrt{2}}$

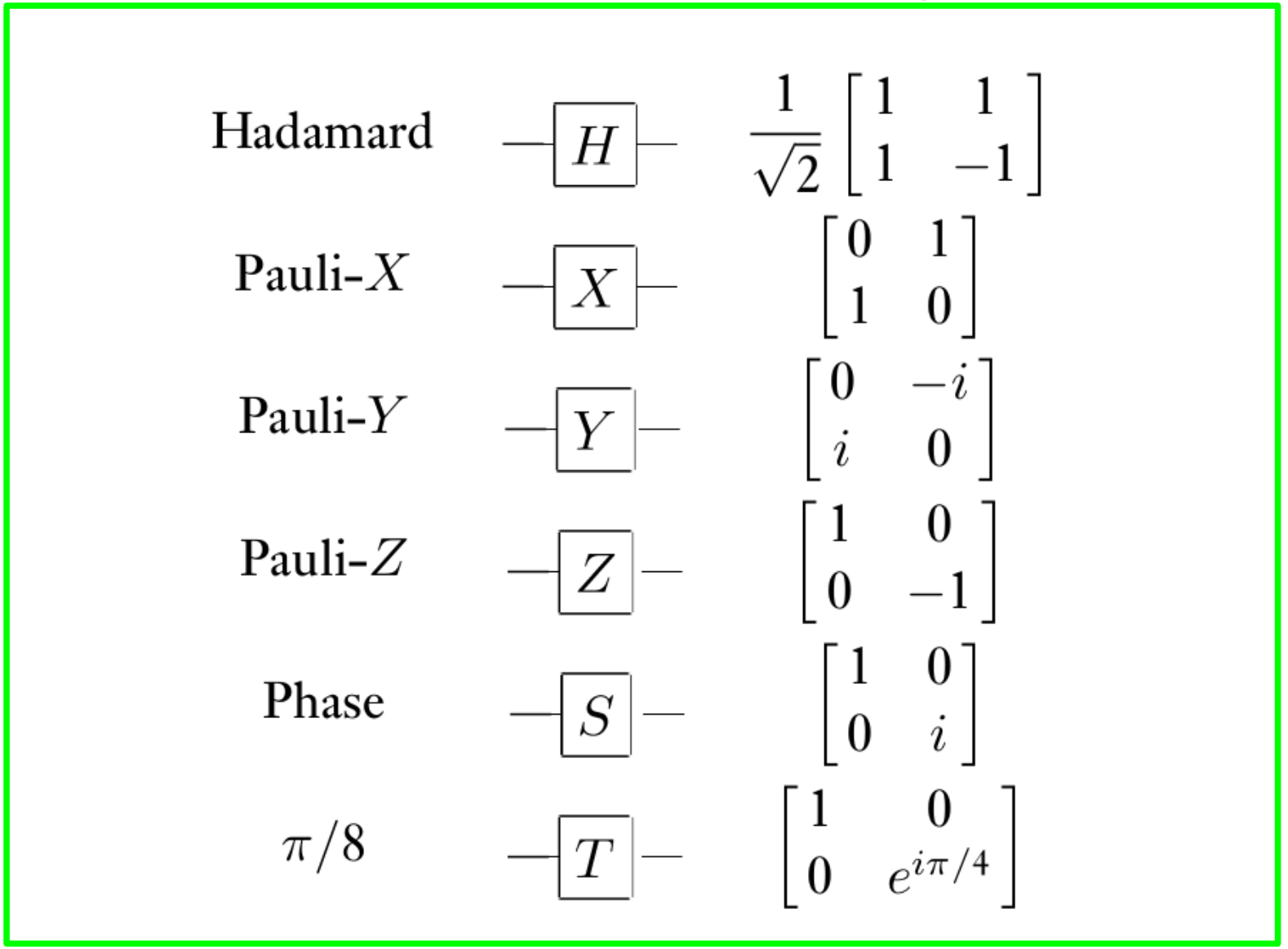
M. A. Nielsen, I. L. Chuang, Quantum Computation and Quantum Information

Classical gates



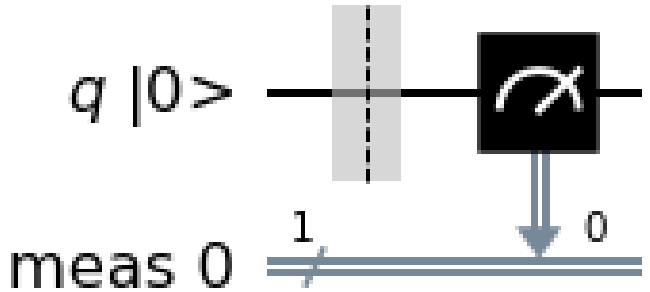
M. A. Nielsen, I. L. Chuang, Quantum Computation and Quantum Information

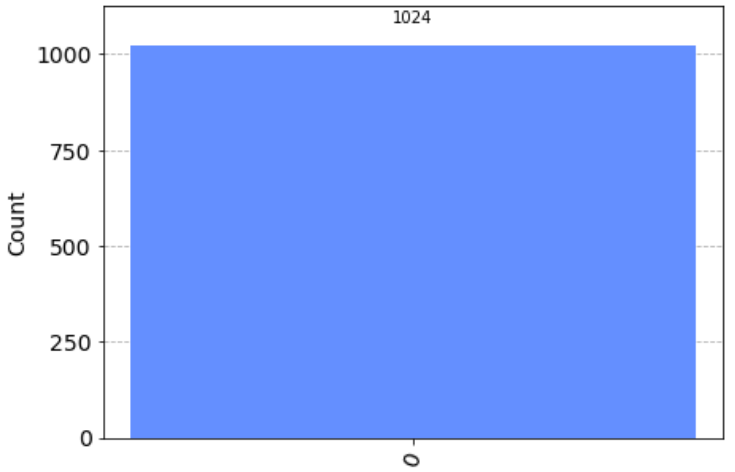
1 qubit quantum gates

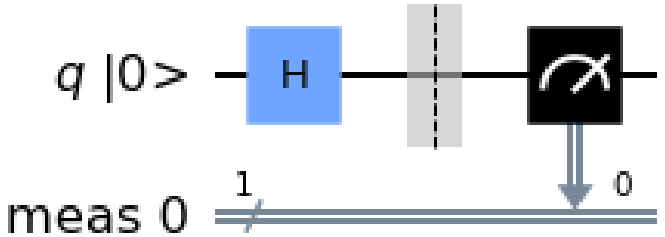


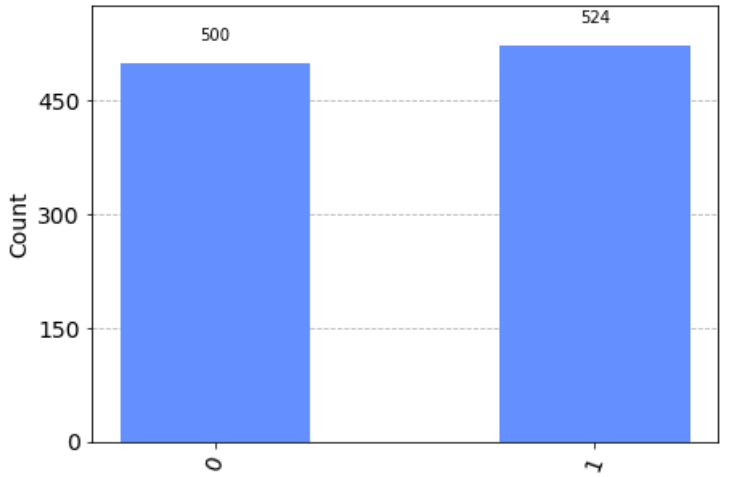
M. A. Nielsen, I. L. Chuang, Quantum Computation and Quantum Information

Some simple circuits









Results from qiskit Qiskit

Why Quantum Computing in Nuclear Physics

- The U.S. Department of Energy in its document Energy Research Opportunity II (2019) establishes "A broad theory program should be supported, which can, e.g., **develop methods to address problems in NP using digital quantum computers and quantum simulators**, **utilize QIS concepts** to better understand nuclear phenomena (such as the nuclear many-body problem andhadronization), and develop new QIS applications of importance to nuclear physics".
- In the future, quantum computers will allow to outperform present computational (classical) capabilities.
- The applications of Quantum Computing in Nuclear Physics are increasing.

First applications in Nuclear Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu, A. J. McCaskey, G. Hagen, G. R. Jansen, T. D. Morris, T. Papenbrock, R. C. Pooser, D. J. Dean, and P. Lougovski

Phys. Rev. Lett. 120, 210501 (2018)

- Quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers.
- Use of a variational wave-function ansatz based on unitary coupled-cluster theory (UCC)→ **Variational Quantum Eigensolver**

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

$$\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\left[(2n+3/2)\delta^{n'}_n - \sqrt{n(n+1/2)}\delta^{n'+1}_n - \sqrt{(n+1)(n+3/2)}\delta^{n'-1}_n\right],$$

$$V_0 = -5.68658111 \text{ MeV}$$

$$\hbar\omega = 7 \text{ MeV}$$

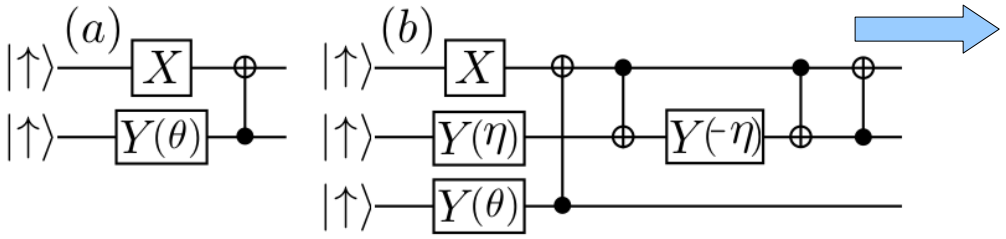
$$\langle n'|V|n\rangle = V_0\delta^0_n\delta^{n'}_n.$$

$$\begin{aligned} H_1 &= 0.218291(Z_0 - I) \\ H_2 &= 5.906709I + 0.218291Z_0 - 6.125Z_1 \\ &\quad - 2.143304\,(X_0X_1 + Y_0Y_1)\,, \\ H_3 &= H_2 + 9.625(I - Z_2) \\ &\quad - 3.913119\,(X_1X_2 + Y_1Y_2)\,. \end{aligned}$$

Jordan-Wigner transformation

Cloud Quantum Computing of an Atomic Nucleus

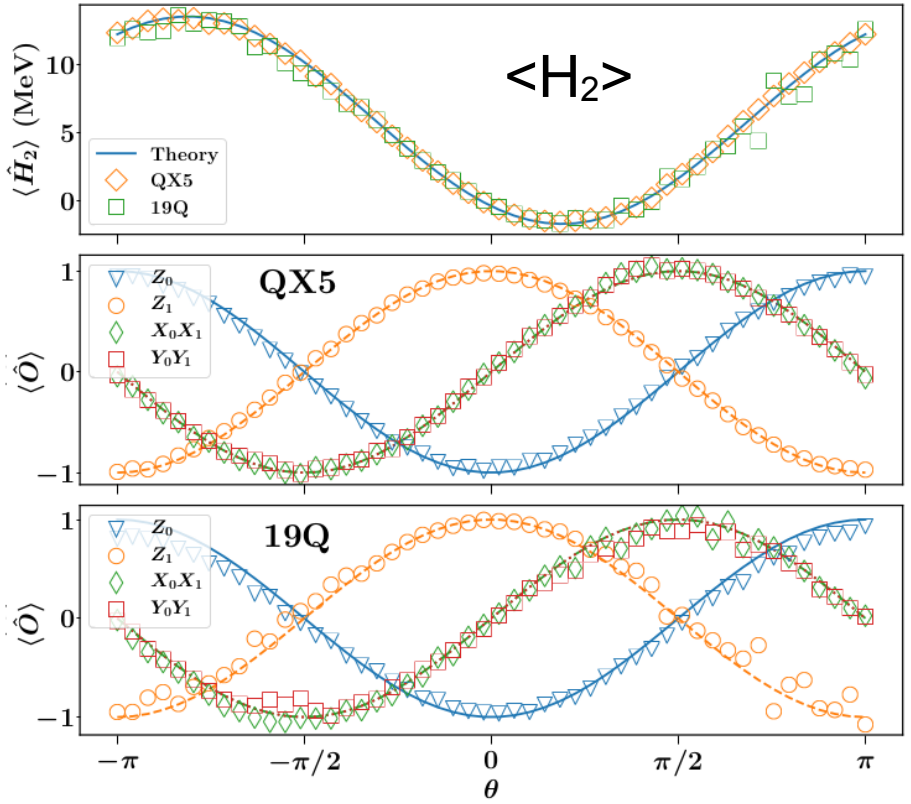
Variational wave function

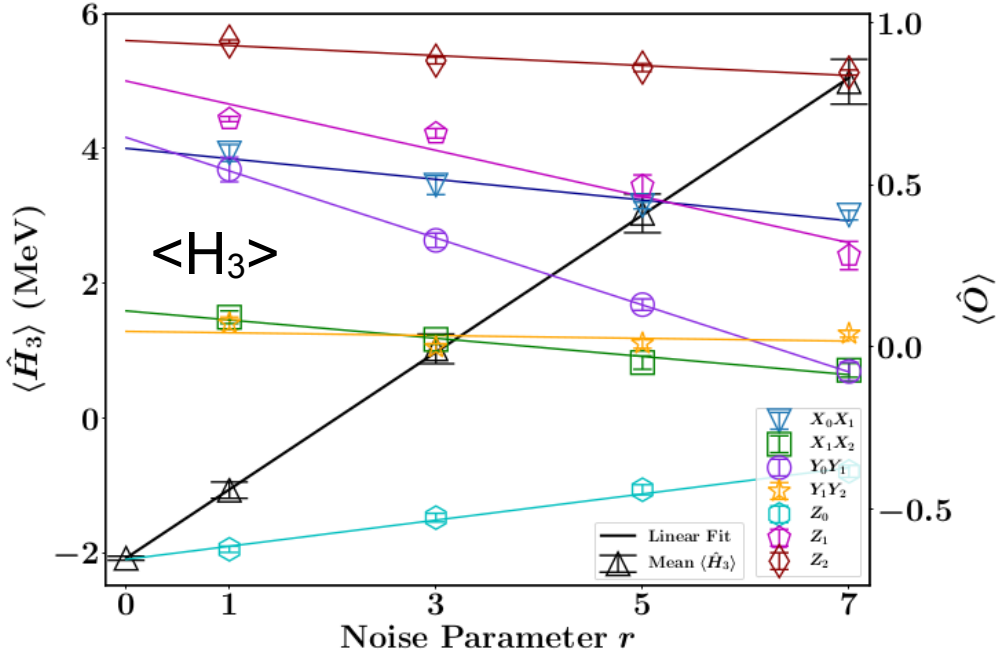


$$U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)},$$

$$U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)+\theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

$$\approx e^{i\frac{\eta}{2}(X_0Y_1 - X_1Y_0)} e^{i\frac{\theta}{2}(X_0Z_1Y_2 - X_2Z_1Y_0)}$$





E(exact)=-2.22 MeV, E(H_2)=-2.18 MeV, E(H_3)=-2.21MeV

The Jordan-Wigner transformation

The transformation

$$c_i^\dagger = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^- \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$

$$c_i = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^+ \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$

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 Variational Quantum Eigensolver (VQE)

nature COMMUNICATIONS

ARTICLE

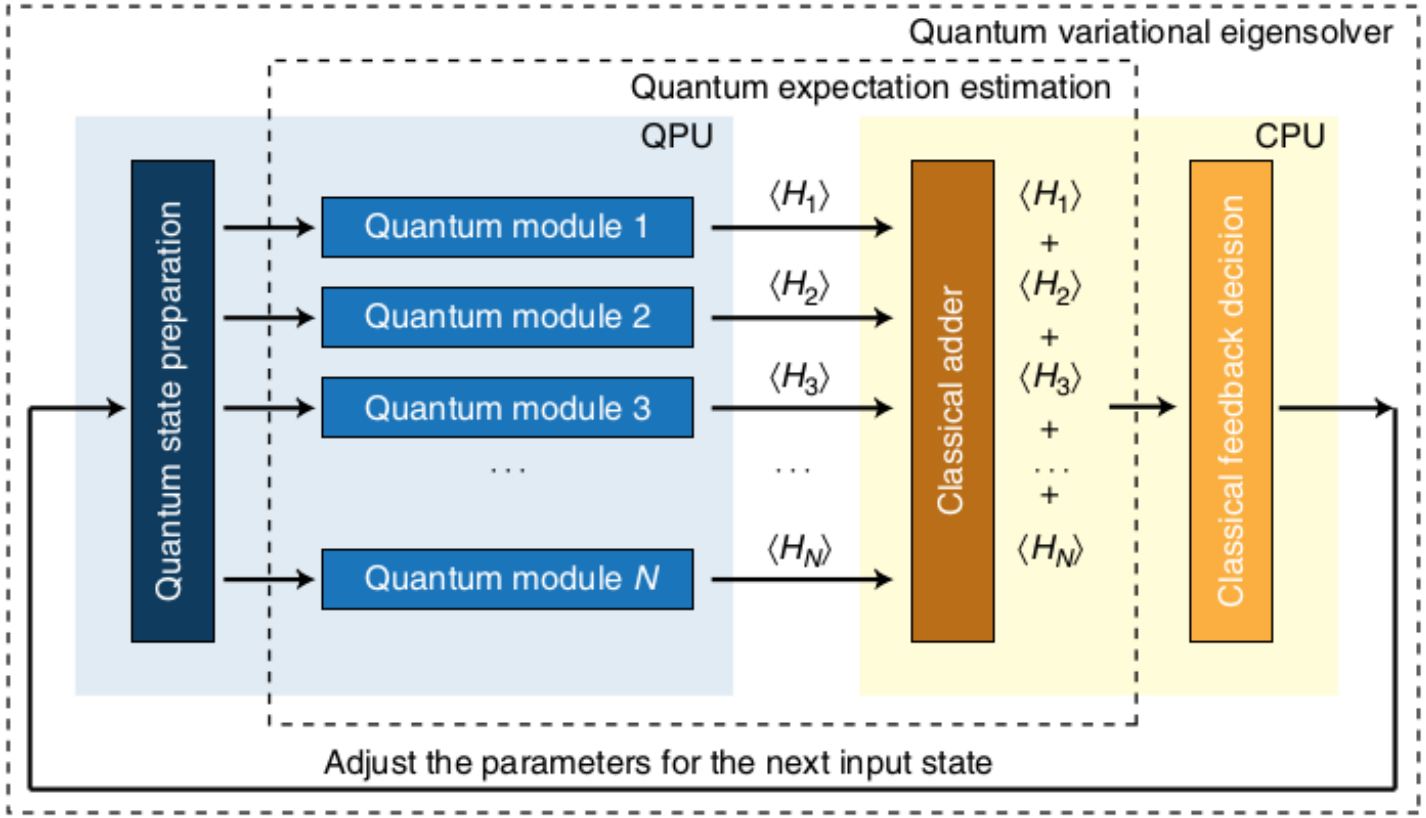
Received 9 Dec 2013 | Accepted 27 May 2014 | Published 23 Jul 2014 DOI: 10.1038/ncomms5213 OPEN

A variational eigenvalue solver on a photonic quantum processor

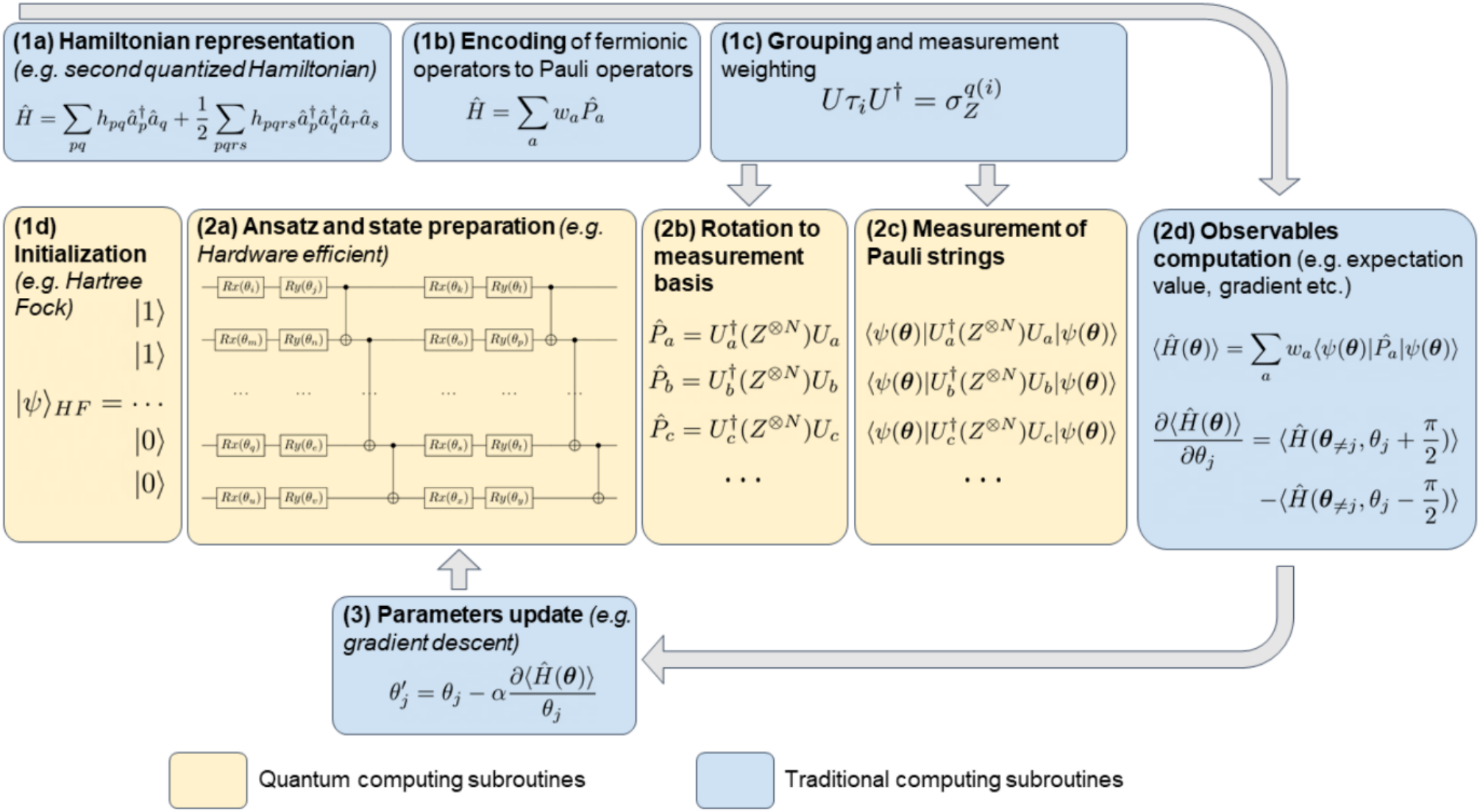
Alberto Peruzzo[1,*,†], Jarrod McClean[2,*], Peter Shadbolt[1], Man-Hong Yung[2,3], Xiao-Qi Zhou[1], Peter J. Love[4], Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]

$$E_0 \leqslant \frac{\langle\psi|\,\hat{H}\,|\psi\rangle}{\langle\psi|\psi\rangle}. \qquad E_{\mathrm{VQE}} = \min_{\theta} \langle \mathbf{0}|\, U^{\dagger}(\theta)\hat{H}U(\theta)\,|\mathbf{0}\rangle .$$

$$\hat{H} = \sum_{a}^{\mathcal{P}} w_a \hat{P}_a, \qquad E_{\mathrm{VQE}} = \min_{\theta} \sum_{a}^{\mathcal{P}} w_a \langle \mathbf{0}|\, U^{\dagger}(\theta)\hat{P}_a U(\theta)\,|\mathbf{0}\rangle ,$$



The Variational Quantum Eigensolver (VQE)



J. Tilly, et al, "The Variational Quantum Eigensolver: A review of methods and best practices", Physics Reports 986, 1 (2022).

Lipkin model on a quantum computer

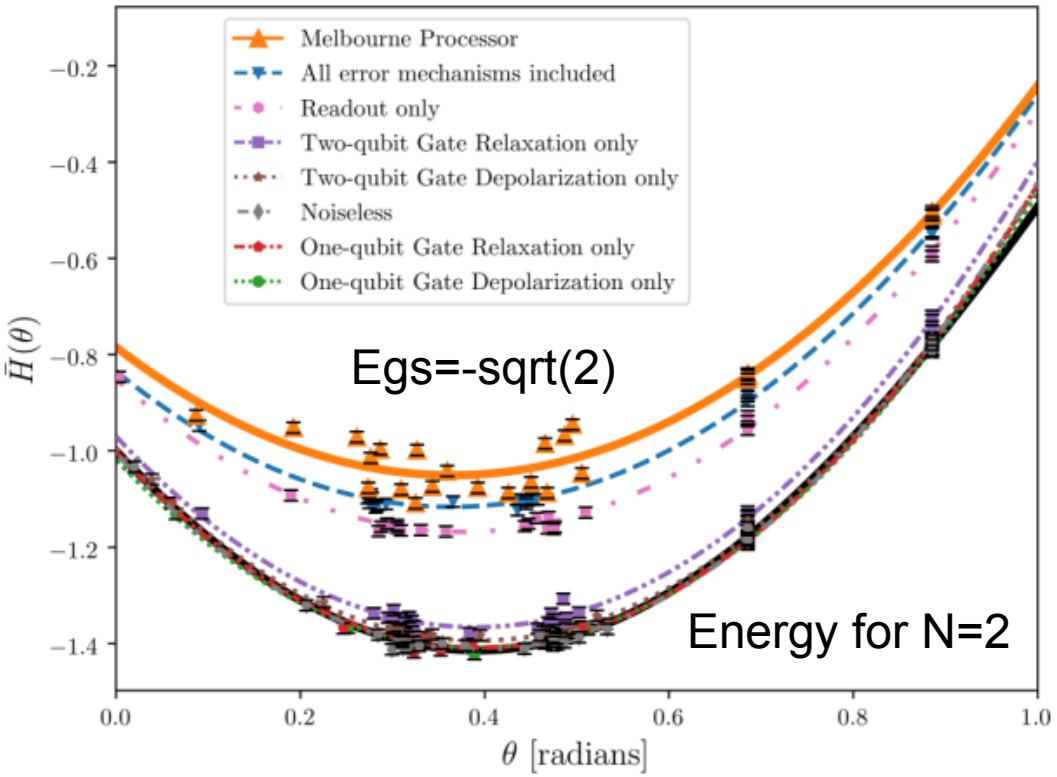
M. J. Cervia, A. B. Balantekin, S. N. Coppersmith, Calvin W. Johnson, Peter J. Love, C. Poole. K. Robbins, and M. Saffman

Physical Review C 104, 024305 (2021)

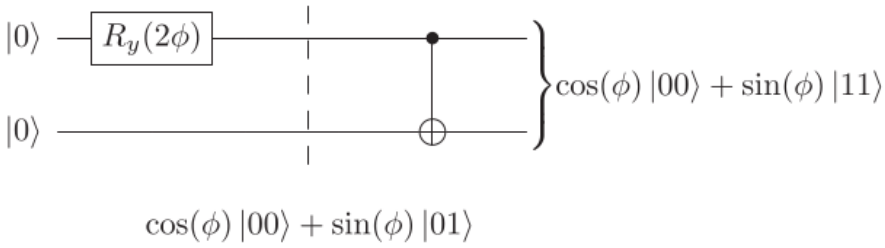
- Quantum simulation of the Lipkin Hamiltonian binding energy on quantum processors accessed via cloud servers.
- Use of a variational wave-function ansatz → **VQE**
- No Jordan-Wigner transformation is needed.

$$H = \sum_{p=1}^{N} J_0^{(p)} + V \sum_{\substack{p,q=1 \\ q \neq p}}^{N} (J_+^{(p)} J_+^{(q)} + J_-^{(q)} J_-^{(p)}).$$

Results for N=**2**, 3, 4

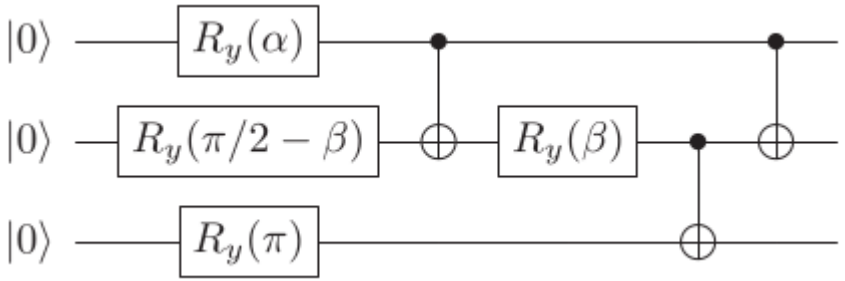


Trial wave function for N=2



$\cos(\phi)\,|00\rangle + \sin(\phi)\,|01\rangle$

Trial wave function for N=3

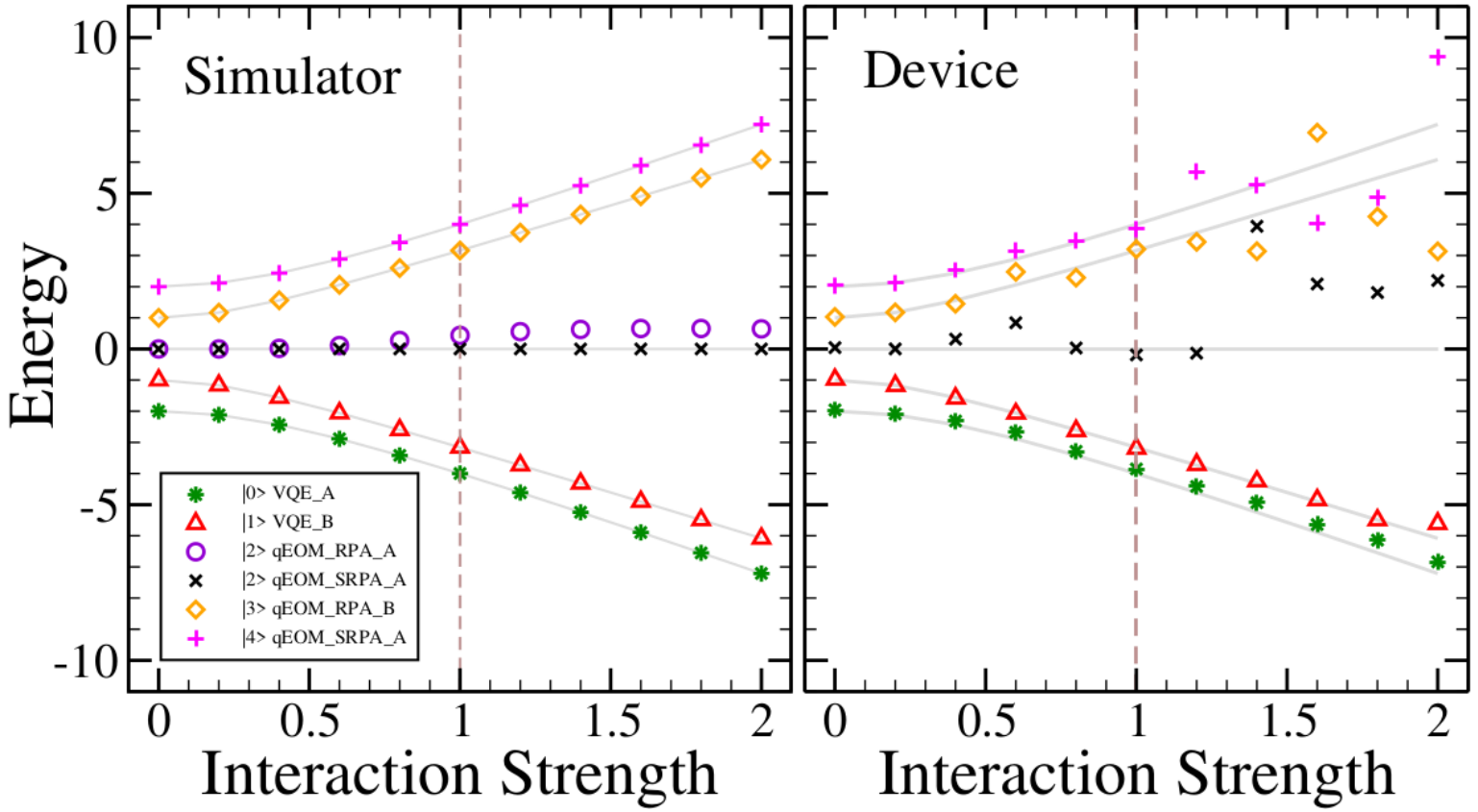


Simulating excited states of the Lipkin model on a quantum computer

Manqoba Q. Hlatshwayo, Yinu Zhang, Herlik Wibowo, Ryan LaRose, Denis Lacroix, and Elena Litvinova

Phys. Rev. C 106, 024319 (2022)

- Quantum simulation of the excited state energies for the Lipkin model.
- Use of the Quantum Equation of Motion (qEOM) method.
- Calculations for N = 2, 3 and 4 particles.
- The accuracy strongly depend on the fermion to qubit encoding.



N=4

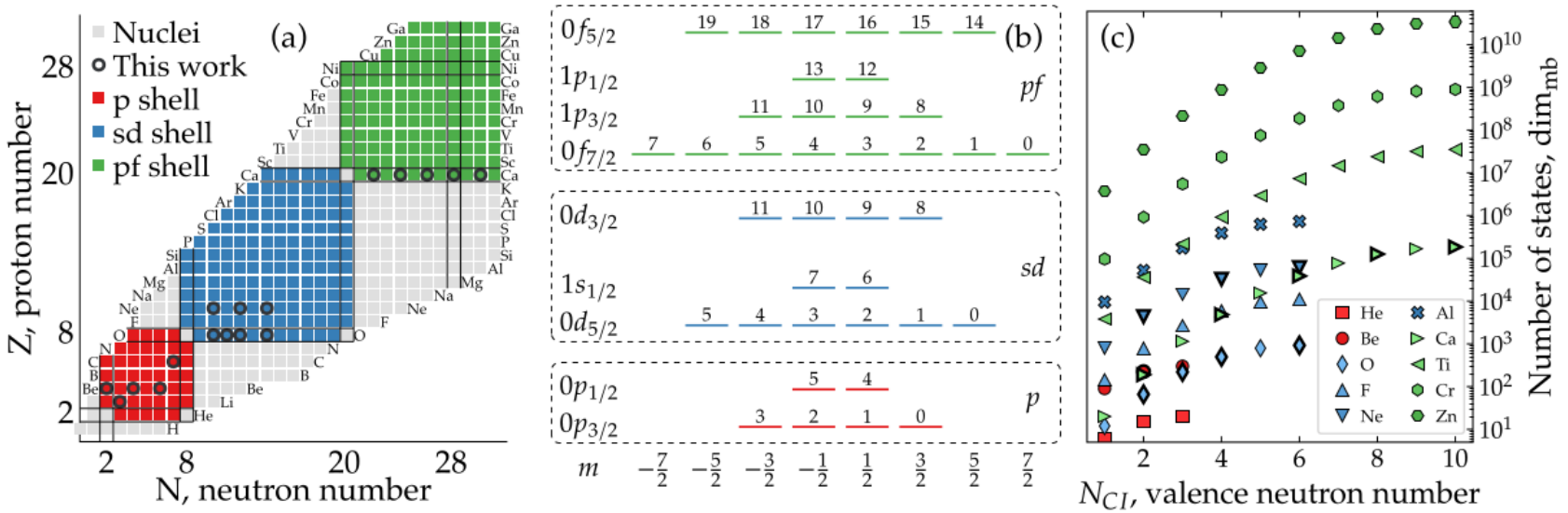
Other selected applications: Shell Model calculations

Nuclear shell-model simulation in digital quantum computers

A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz

Scientific Reports 13:12291 (2023)

- Use of the adaptive variational quantum eigensolver algorithm (ADAPT-VQE).
- Calculation of the ground state energy in the p, sd, and pf shells.



Shell	N_{qb}	N_h	N_{hh}	N_{tot}
p	6	2	10 (9)	13 (12)
	12	4	109 (44)	114 (49)
sd	12	8	203 (86)	212 (95)
	24	16	1389 (518)	1406 (535)
pf	20	20	1507 (570)	1528 (591)
	40	40	10,572 (3459)	10,613 (3500)

Number of circuits

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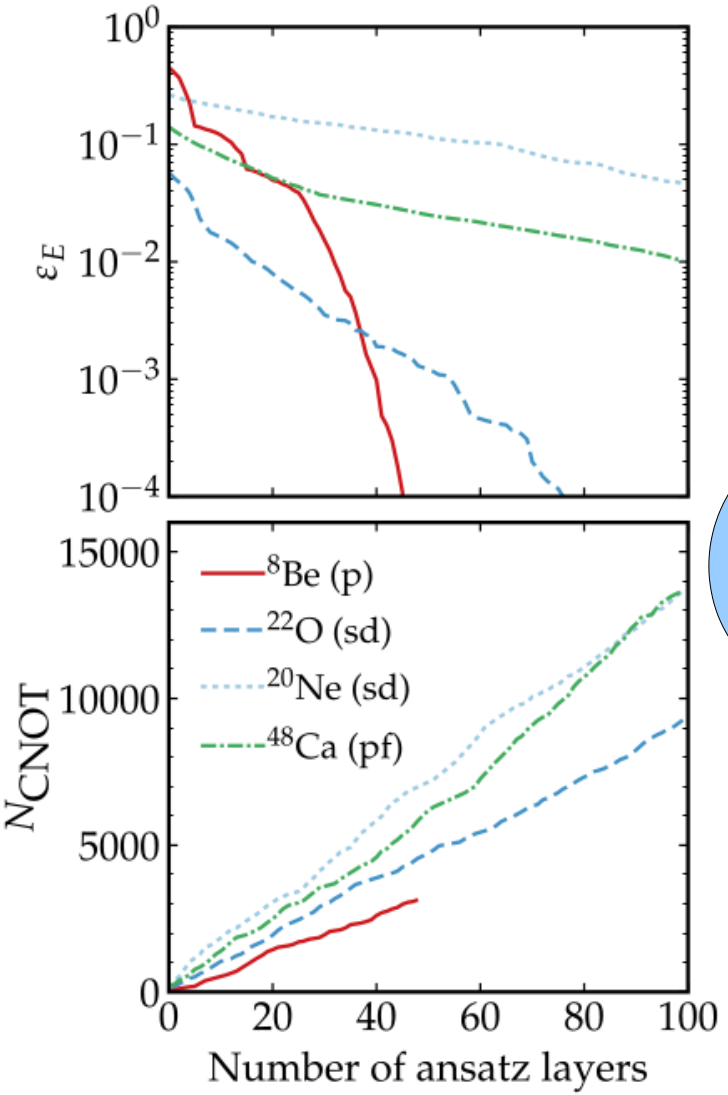
Scientific Reports 13:12291 (2023)

Accuracy and number of CNOTs



ADAPT-VQE method

$$|\psi(\boldsymbol{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k} |\mathrm{ref}\rangle, \qquad |\psi(\boldsymbol{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k} |\mathrm{ref}\rangle,$$

$$\left.\frac{\partial E^{(n)}}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\boldsymbol{\theta})|[H_{\mathrm{eff}}, A_k]|\psi(\boldsymbol{\theta})\rangle|_{\theta_k=0}$$

The new operator is selected according to the largest energy gradient

Pool of operators: $T^{pq}_{rs} = i(a^\dagger_p a^\dagger_q a_r a_s - a^\dagger_r a^\dagger_s a_p a_q)$

Nuclear shell-model simulation in digital quantum computers

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Scientific Reports 13:12291 (2023)

	Fermion operators	Qubit operators
n_p	$a_p^\dagger a_p$	$\frac{1}{2}(1 - Z_p)$
h_{pqrs}	$a_p^\dagger a_q^\dagger a_r a_s + a_r^\dagger a_s^\dagger a_p a_q$	$\frac{1}{8} P_{rs}^{pq} (-X_p X_q X_r X_s + X_p X_q Y_r Y_s - X_p Y_q X_r Y_s - X_p Y_q Y_r X_s - Y_p Y_q Y_r Y_s + Y_p Y_q X_r X_s - Y_p X_q Y_r X_s - Y_p X_q X_r Y_s)$
T_{rs}^{pq}	$i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$	$\frac{1}{8} P_{rs}^{pq} (-X_p Y_q Y_r Y_s - Y_p X_q Y_r Y_s + Y_p Y_q X_r Y_s + Y_p Y_q Y_r X_s + Y_p X_q X_r X_s + X_p Y_q X_r X_s - X_p X_q Y_r X_s - X_p X_q X_r Y_s)$
h_{pq}	$a_p^\dagger a_q + a_q^\dagger a_p$	$\frac{1}{2}\left(\prod_{n=p+1}^{q-1} Z_n\right)(X_p X_q + Y_q Y_p)$
T_{pq}	$i(a_p^\dagger a_q - a_q^\dagger a_p)$	$\frac{1}{2}\left(\prod_{n=p+1}^{q-1} Z_n\right)(Y_p X_q - X_q Y_p)$

$$a_i^\dagger = \left(\prod_{k=0}^{i-1} Z_k\right)\sigma_i^-, \quad a_i = \left(\prod_{k=0}^{i-1} Z_k\right)\sigma_i^+$$

$$P_{rs}^{pq} \equiv \left(\prod_{m=p+1, m\notin[r,s]}^{q-1} Z_m\right)\left(\prod_{n=r+1, n\notin[p,q]}^{s-1} Z_n\right)$$

Nuclear shell-model simulation in digital quantum computers

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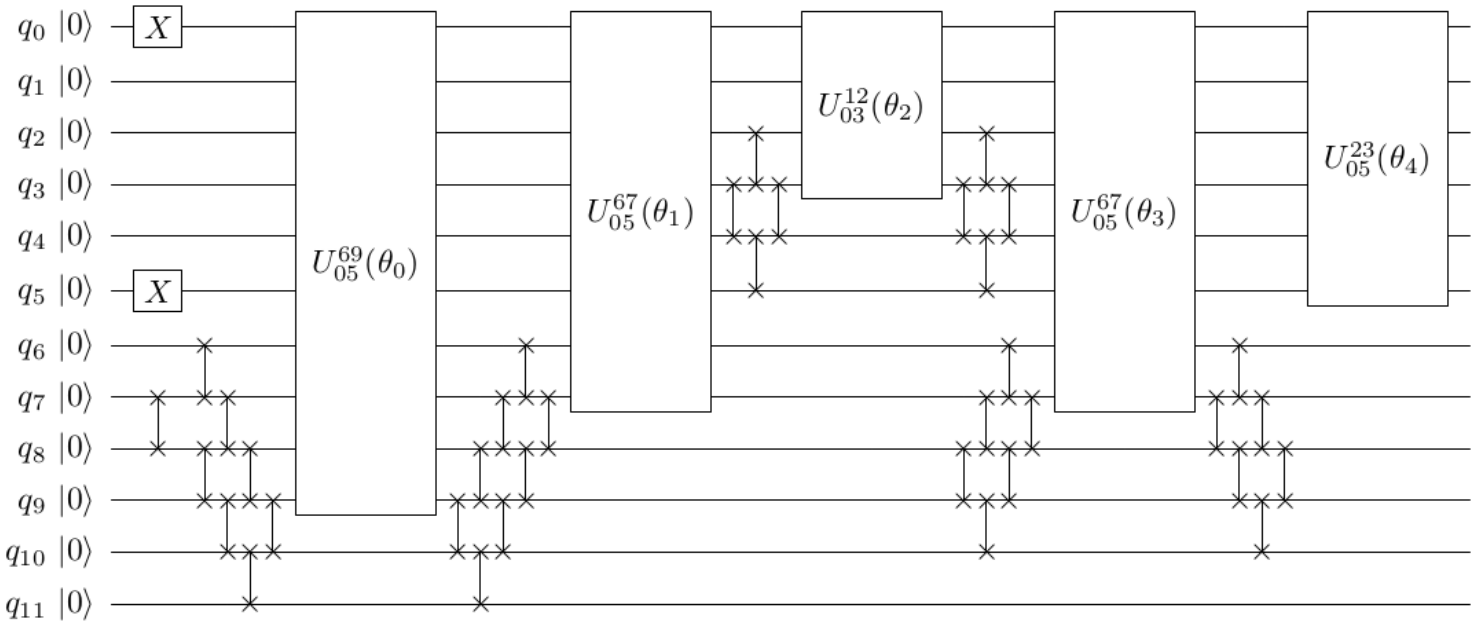
Scientific Reports 13:12291 (2023)

Circuit for ^{18}O



The measurements

$$\langle\psi_n|n_i|\psi_n\rangle = \frac{1}{2}\langle\psi_n|1 - Z_i|\psi_n\rangle = p_1^{(i)} \qquad \langle\psi_n|h_{ijij}|\psi_n\rangle = -2\langle\psi_n|n_i n_j|\psi_n\rangle = -2p_{11}^{(ij)}$$

$$\langle\psi_n|h_{ijik}|\psi_n\rangle = p_{101}^{(ijk)} - p_{110}^{(ijk)} \qquad \langle\psi_n|h_{ijik}|\psi_n\rangle = p_{101}^{(ijk)} - p_{110}^{(ijk)}$$

Other selected applications: Phase diagram of the Agassi model

A digital quantum simulation of the Agassi model,

P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

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

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

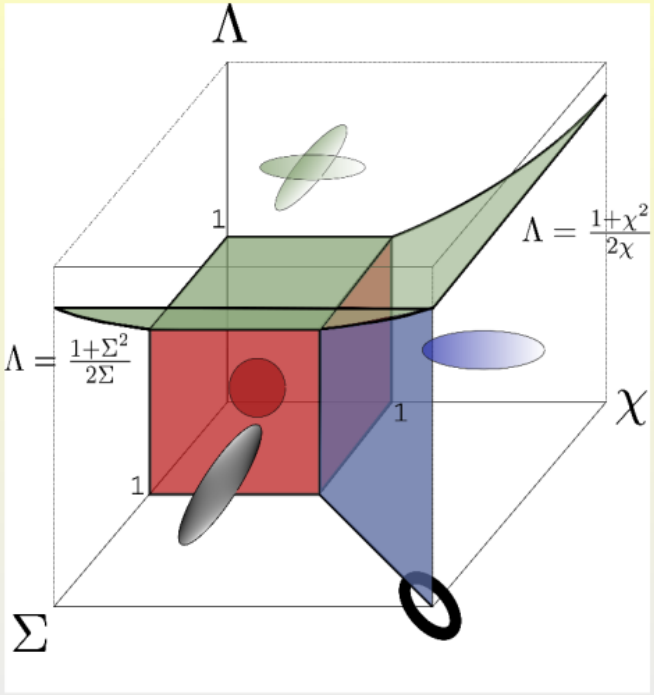
$\sigma = +1, -1$ and $m = -j, \ldots, -2, -1, 1, 2, \ldots, j$. Degeneracy $\Omega = 2j$

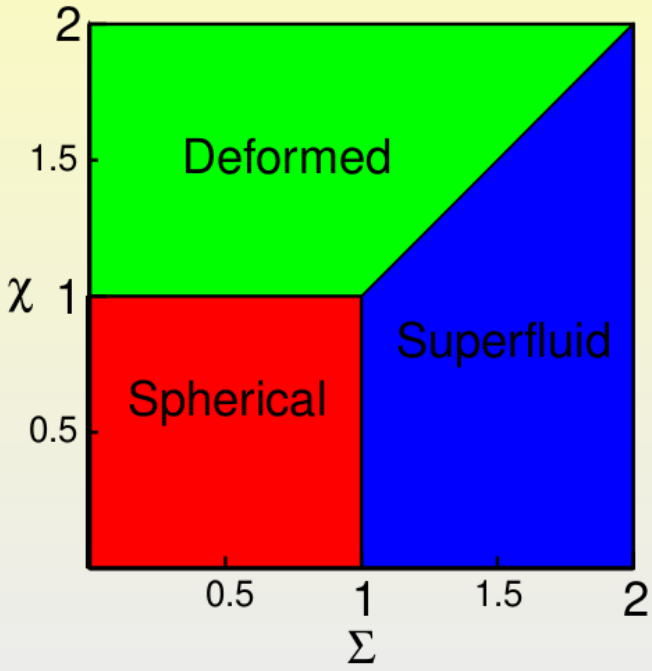
A digital quantum simulation of the Agassi model,

P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,

Physics Letters B 829, 137133 (2022).

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))

A digital quantum simulation of the Agassi model,

P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

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.

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.

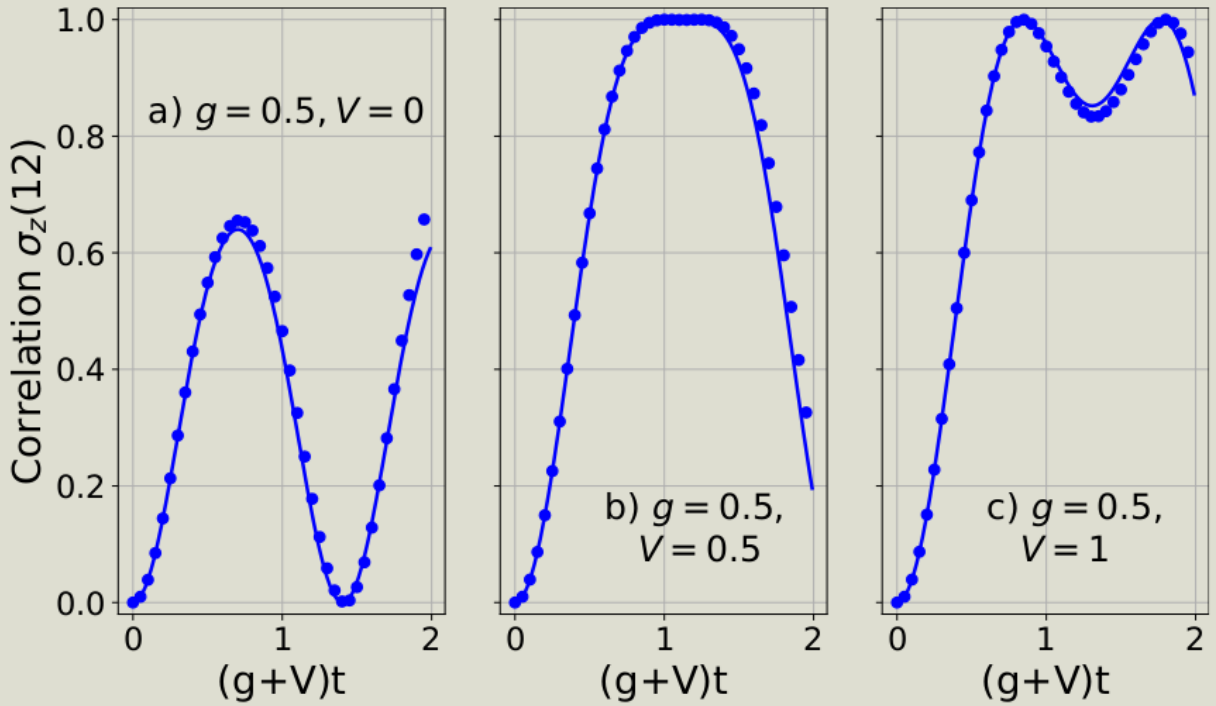
A digital quantum simulation of the Agassi model,

P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

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).

A digital quantum simulation of the Agassi model,

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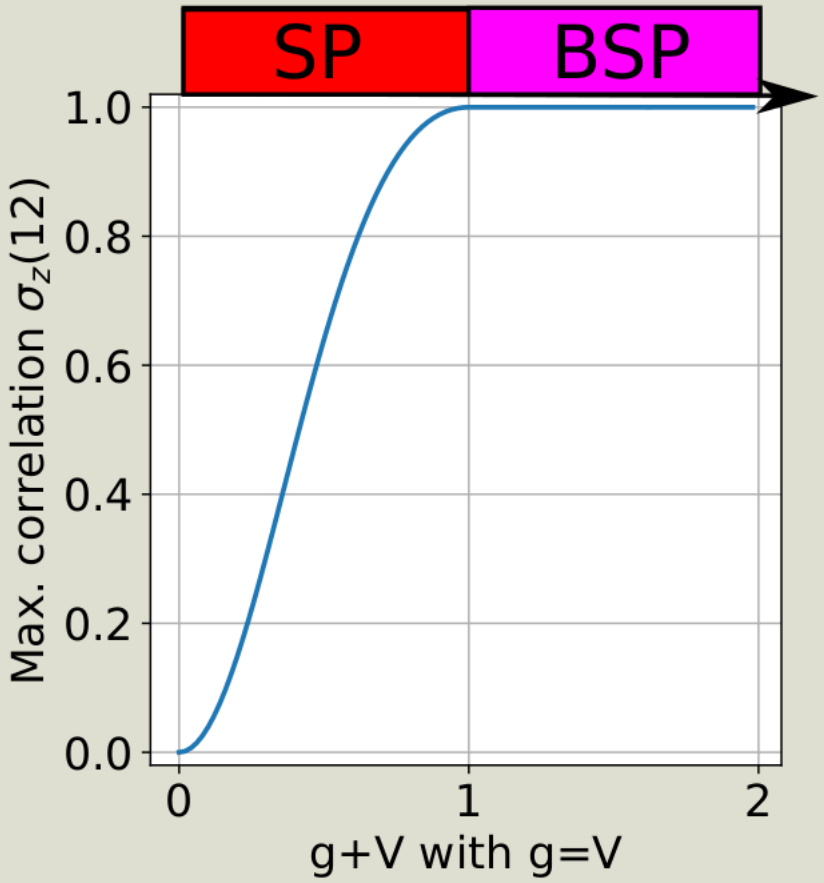
Physics Letters B 829, 137133 (2022).

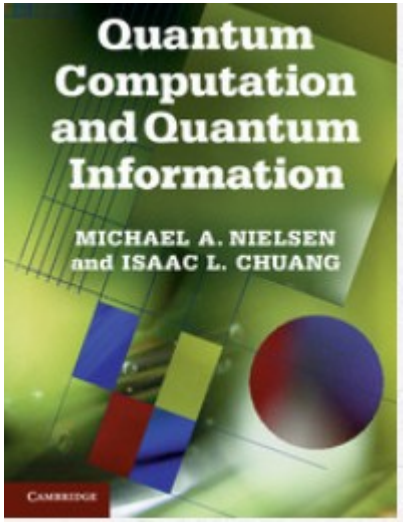
Is it possible to determine the phase of the system?

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



Still interested?
Really willing to start with QC?

To start with



PHYSICAL REVIEW A, VOLUME 65, 042323

Simulating physical phenomena by quantum networks

R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 12 September 2001; published 9 April 2002)

Physical systems, characterized by an ensemble of interacting constituents, can be represented and studied by different algebras of operators (observables). For example, a fully polarized electronic system can be studied by means of the algebra generated by the usual fermionic creation and annihilation operators or by the algebra of Pauli (spin-1/2) operators. The Jordan-Wigner isomorphism gives the correspondence between the two algebras. As we previously noted, similar isomorphisms enable one to represent any physical system in a quantum computer. In this paper we evolve and exploit this fundamental observation to simulate generic physical phenomena by quantum networks. We give quantum circuits useful for the efficient evaluation of the physical properties (e.g., the spectrum of observables or relevant correlation functions) of an arbitrary system with Hamiltonian H.

Interested in doing calculations?

Qiskit https://qiskit.org/, https://quantum.ibm.com/

Cirq https://quantumai.google/cirq

OpenFermion https://quantumai.google/openfermion

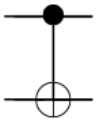
(Personal) Conclusions

- Quantum Computing in Nuclear Physics is still in its infancy, specially if compared with Molecular Physics.
- The calculations that can be afforded today can be easily done in a standard HPC cluster, if not in a laptop.
- There is a lot of room for the implementation and design of new algorithms in Quantum Computing.
- The use of Quantum Computing and Quantum Information techniques can strongly contribute to the development of new "classical" Nuclear Structure ideas.

Thank you

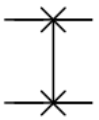
2 qubits quantum gates

controlled-NOT



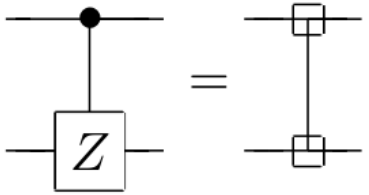
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

swap



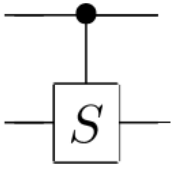
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

controlled-Z



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

controlled-phase



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}$$

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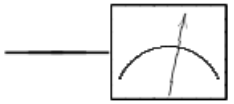
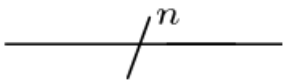
Other elements

measurement		Projection onto $\|0\rangle$ and $\|1\rangle$
qubit		wire carrying a single qubit (time goes left to right)
classical bit		wire carrying a single classical bit
n qubits		wire carrying n qubits

$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} Z = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}.$$

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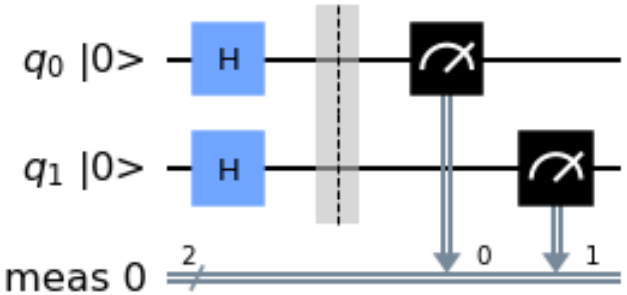
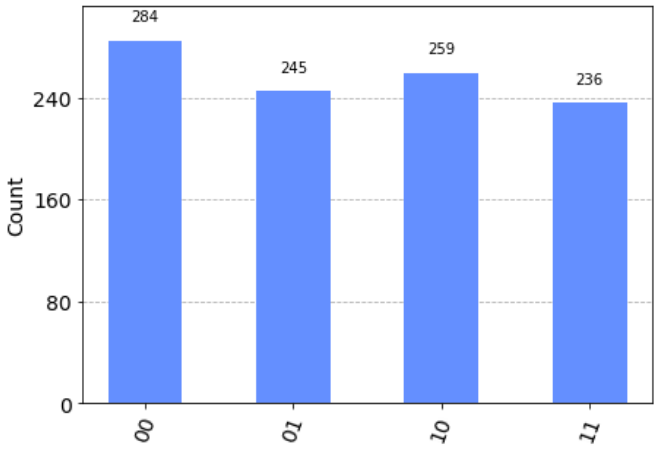
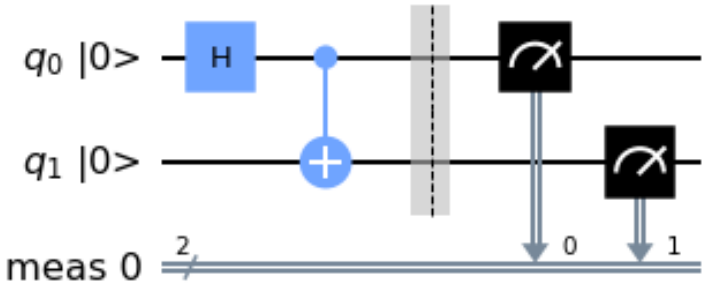
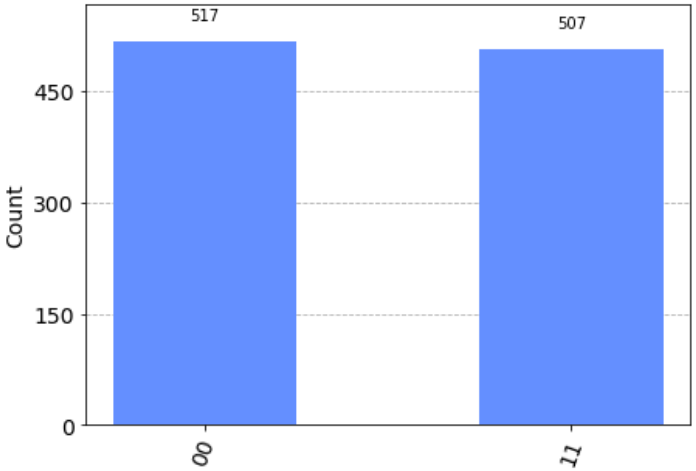
A step further







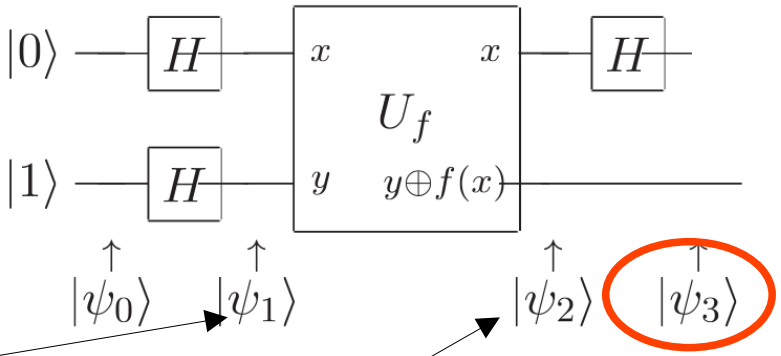


Results from qiskit Qiskit

Deutsch's algorithm

Let us a function, f: {0,1} → {0,1}

Problem: to calculate whether
f(0)=f(1) or f(0)≠f(1)



$$|\psi_1\rangle = \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

$$|\psi_2\rangle = \begin{cases} \pm\left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) = f(1) \\ \pm\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) \neq f(1). \end{cases}$$

$$(-1)^{f(x)}|x\rangle(|0\rangle - |1\rangle)/\sqrt{2}$$

$$|\psi_3\rangle = \begin{cases} \pm|0\rangle\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) = f(1) \\ \pm|1\rangle\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) \neq f(1). \end{cases}$$

$$|\psi_3\rangle = \pm|f(0) \oplus f(1)\rangle\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

With a single measurement we solve the problem, while classically we need two measurements!!
|q0> = |0> → **f(0)=f(1)**
|q1> = |1> → **f(0)≠f(1)**

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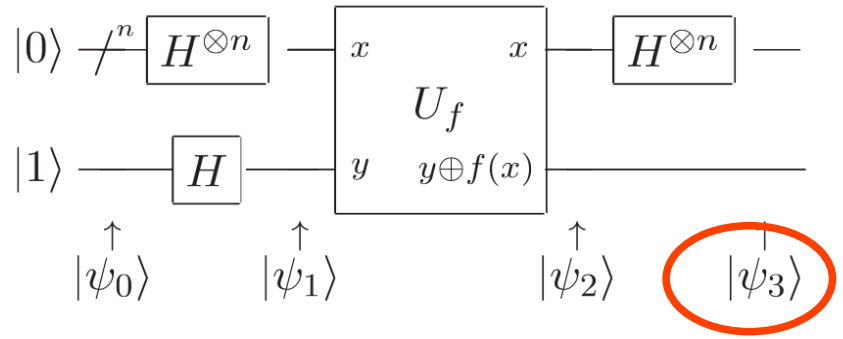
The Deutsch–Jozsa algorithm

Let us a function, f: $[0,2^n-1] \rightarrow \{0,1\}$
Problem: is it the function perfectly balanced or is it constant?



$$|0\rangle^{\otimes n}|1\rangle$$

$$|\psi_1\rangle = \sum_{x\in\{0,1\}^n} \frac{|x\rangle}{\sqrt{2^n}} \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

$$|\psi_2\rangle = \sum_{x} \frac{(-1)^{f(x)}|x\rangle}{\sqrt{2^n}} \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

$$H^{\otimes n}|x_1,\ldots,x_n\rangle = \frac{\sum_{z_1,\ldots,z_n}(-1)^{x_1z_1+\cdots+x_nz_n}|z_1,\ldots,z_n\rangle}{\sqrt{2^n}} \qquad H^{\otimes n}|x\rangle = \frac{\sum_z(-1)^{x\cdot z}|z\rangle}{\sqrt{2^n}}$$

$$|\psi_3\rangle = \sum_z \sum_x \frac{(-1)^{x\cdot z+f(x)}|z\rangle}{2^n} \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

For f constant: probability of measuring $|0\rangle^{\otimes n}$ is one
For f balanced: probability of measuring $|0\rangle^{\otimes n}$ is zero
With a single measurement we solve the problem, while classically we need two $2^n/2+1$ measurements!!

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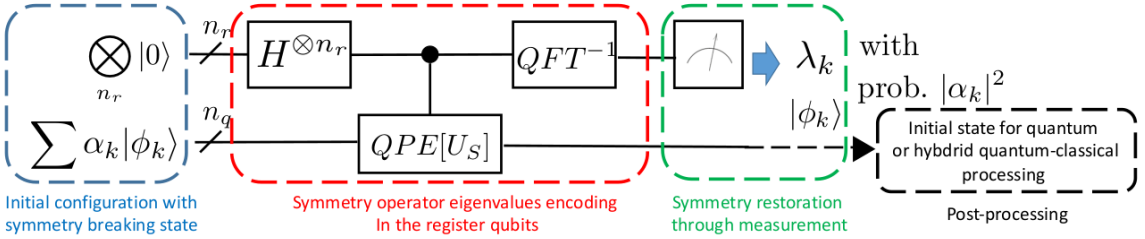
Symmetry-Assisted Preparation of Entangled Many-Body States on a Quantum Computer

Denis Lacroix

Phys. Rev. Lett. 125, 230502 (2020)

- Use of the Quantum Phase Estimation (QPE) algorithm, to construct entangled states that describe correlated many-body systems on quantum computers
- The QPE approach is followed by measurements that serve as projectors on the entangled states.
- The approach can be seen as a quantum–computer formulation of symmetry breaking followed by symmetry restoration.

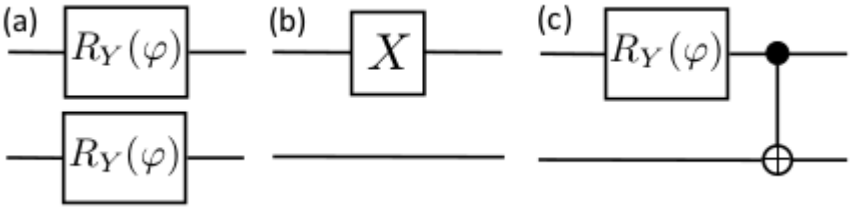


$$H_{\rm P} = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) - g \sum_{i,j>0} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j .$$

$$E/g = -\frac{1}{4}(A-\nu)(2n_q - A - \nu - 2)$$

$$|\psi\rangle = \prod_{n>0} e^{i\varphi(X_n Y_{n+1} + Y_n X_{n+1})/2} |-\rangle \quad \Rightarrow \quad |\psi\rangle = \prod_n \left[\cos\left(\frac{\varphi}{2}\right) I_n \otimes I_{n+1} + \sin\left(\frac{\varphi}{2}\right) Q_n^+ Q_{n+1}^+\right] |-\rangle$$

This state is obtained by applying this circuit to all (n, n + 1) pairs.



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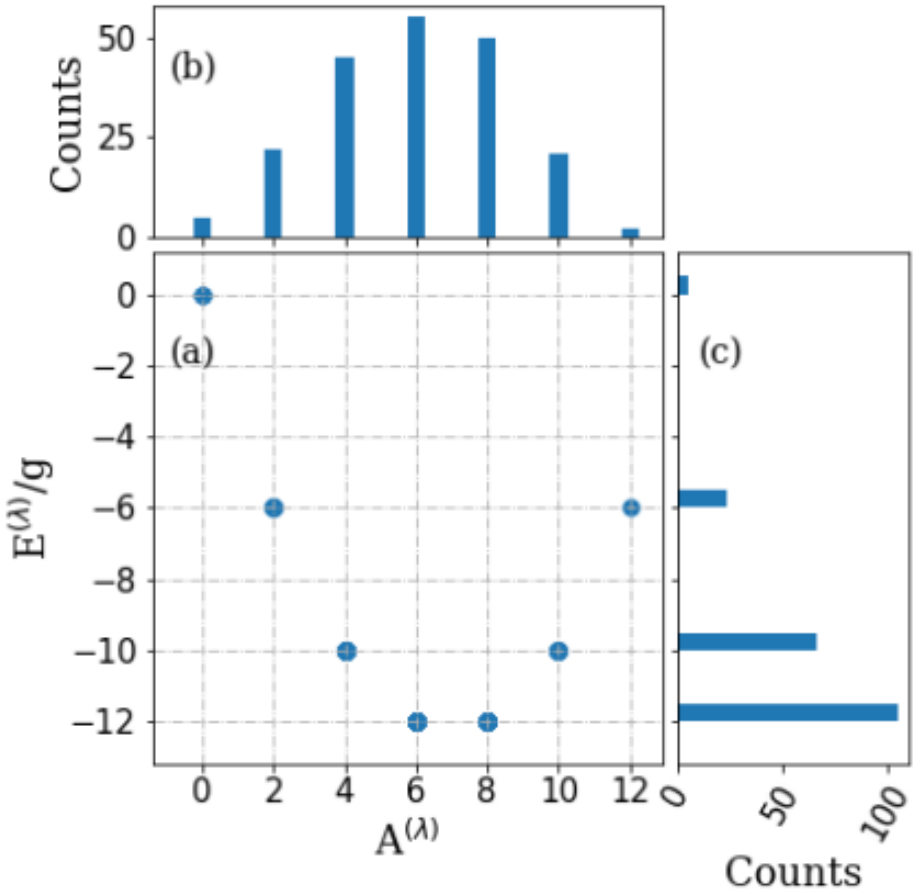
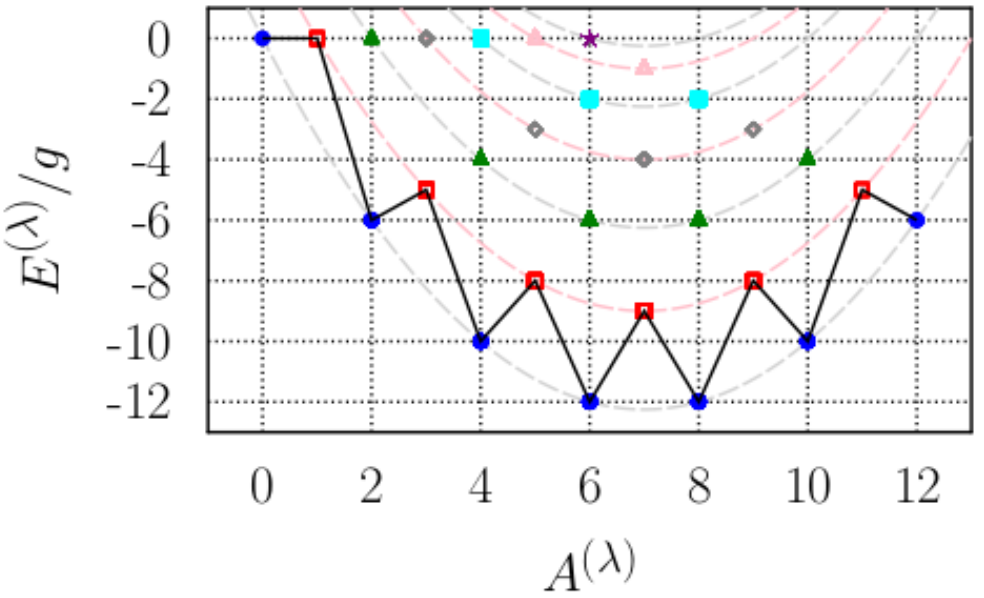




Complete spectrum obtained for n = 12

Correlation between the energies and the particle number. The distribution of counts for the particle number and energies are shown respectively in panels (b) and (c).

Agassi model

The O(5) as the spectrum generator algebra

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

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

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

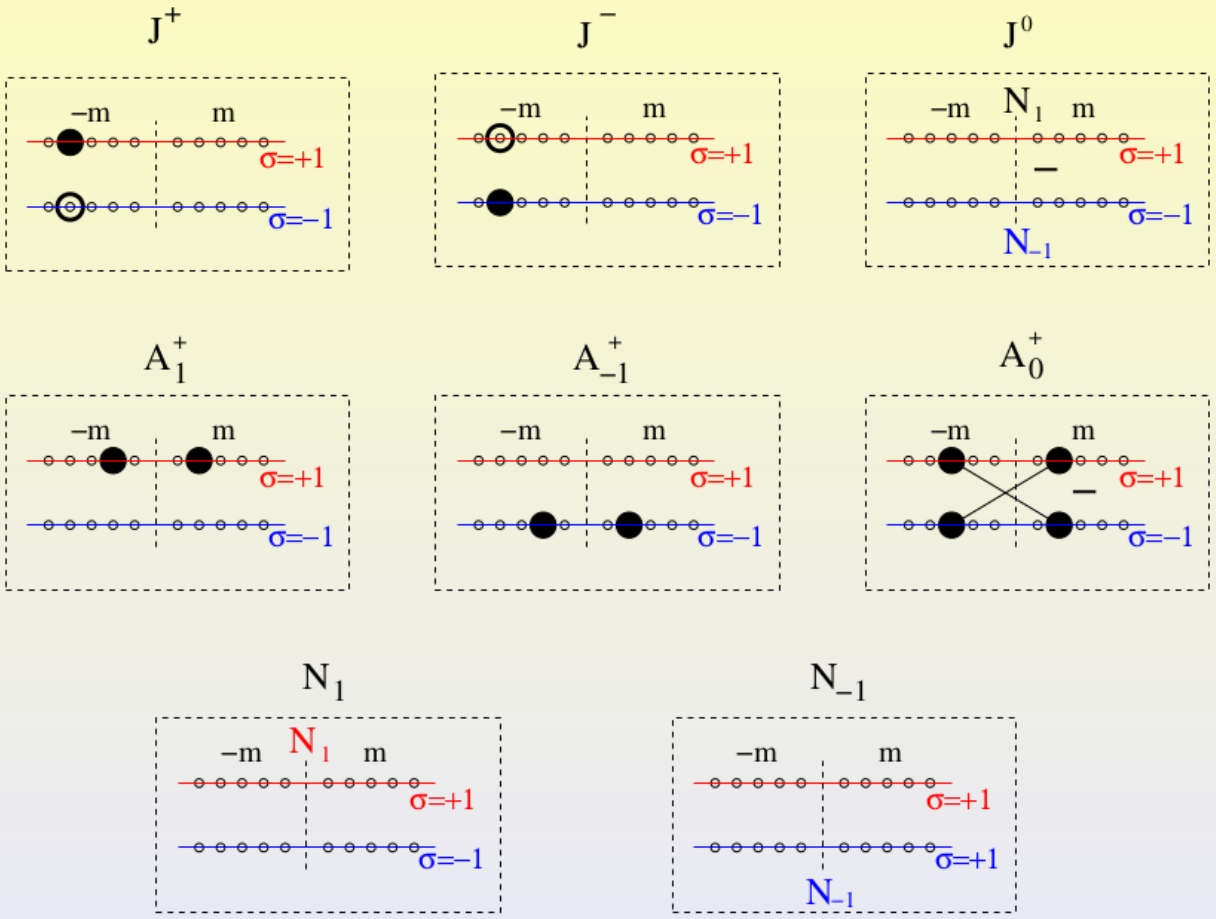
The Hamiltonian

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

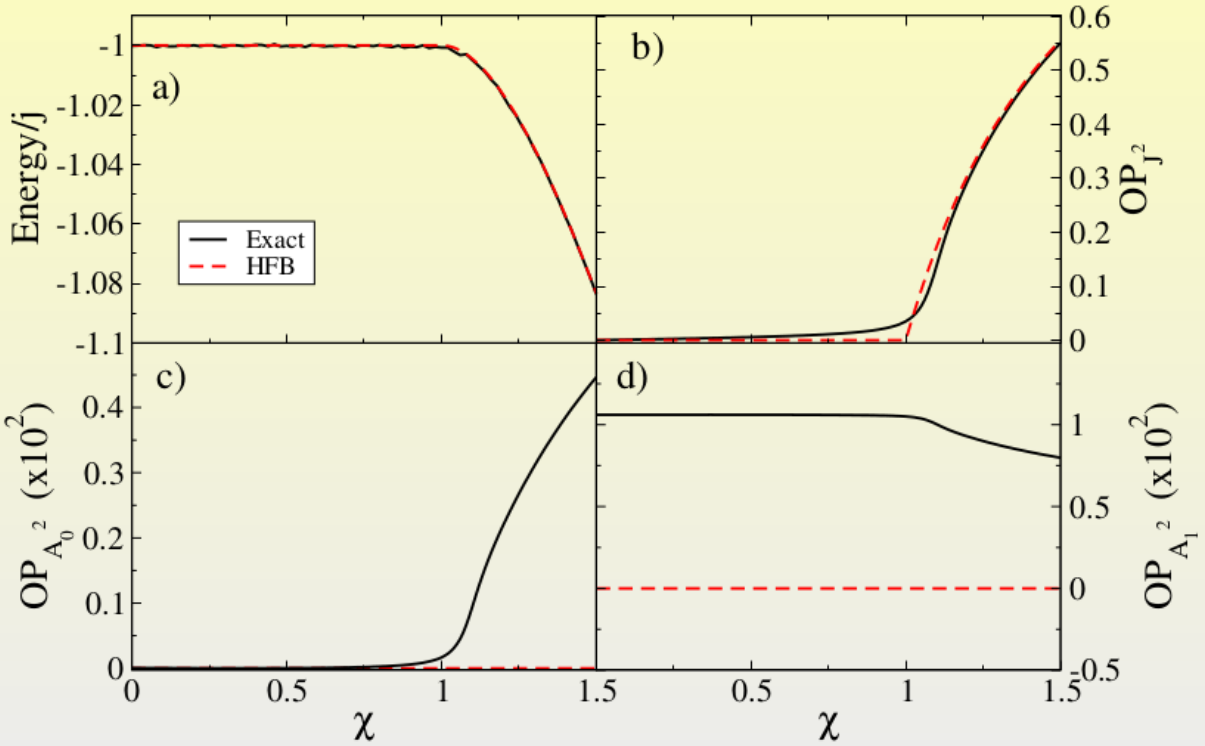
For convenience

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

A pictorial view



Numerical calculations



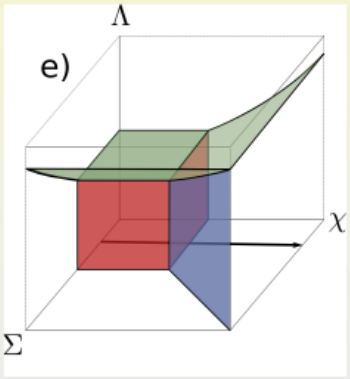
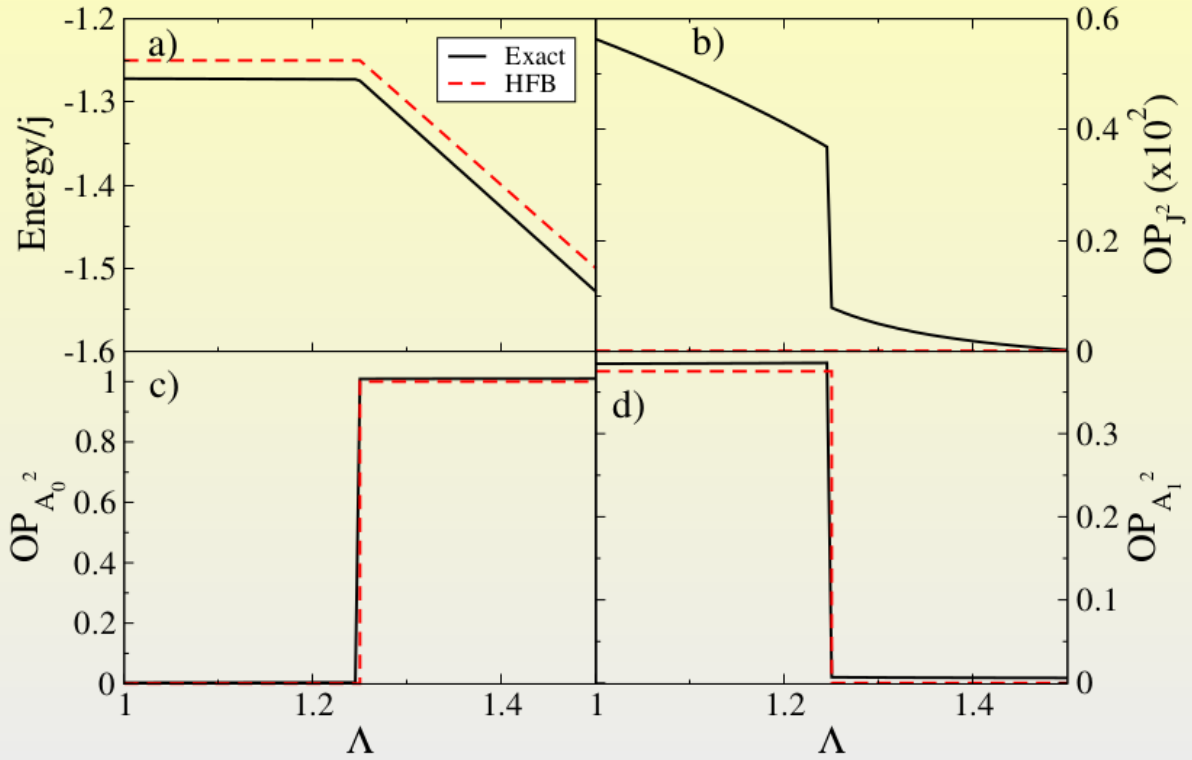


Figure: Comparison of HFB and exact results. $j = 100$ and Hamiltonian parameters $\Sigma = 0.5, \Lambda = 0$.

Numerical calculations



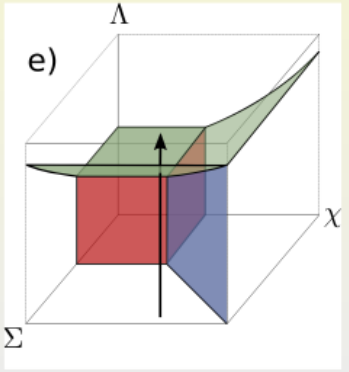


Figure: Comparison of HFB and exact results. $j = 100$ and Hamiltonian parameters $\chi = 1.5, \Sigma = 2$.

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

$$c_i^\dagger = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^- \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$
$$c_i = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^+ \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$

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

$$
\begin{aligned}
c_{1,1} &\rightarrow c_1, \\
c_{1,-1} &\rightarrow c_2, \\
c_{-1,1} &\rightarrow c_3, \\
c_{-1,-1} &\rightarrow c_4.
\end{aligned}
\qquad
\begin{aligned}
J^+ &= -\sigma_2^+ \otimes \sigma_3^z \otimes \sigma_4^- - \sigma_1^+ \otimes \sigma_2^z \otimes \sigma_3^-, \\
J^0 &= (1/4)(\sigma_1^z + \sigma_2^z - \sigma_3^z - \sigma_4^z), \\
J^- = (J^+)^\dagger &= -\sigma_2^- \otimes \sigma_3^z \otimes \sigma_4^+ - \sigma_1^- \otimes \sigma_2^z \otimes \sigma_3^+, \\
A_1^\dagger &= \sigma_1^+ \otimes \sigma_2^+, \; A_{-1}^\dagger = \sigma_3^+ \otimes \sigma_4^+, \\
A_1 &= \sigma_1^- \otimes \sigma_2^-, \; A_{-1} = \sigma_3^- \otimes \sigma_4^-.
\end{aligned}
$$

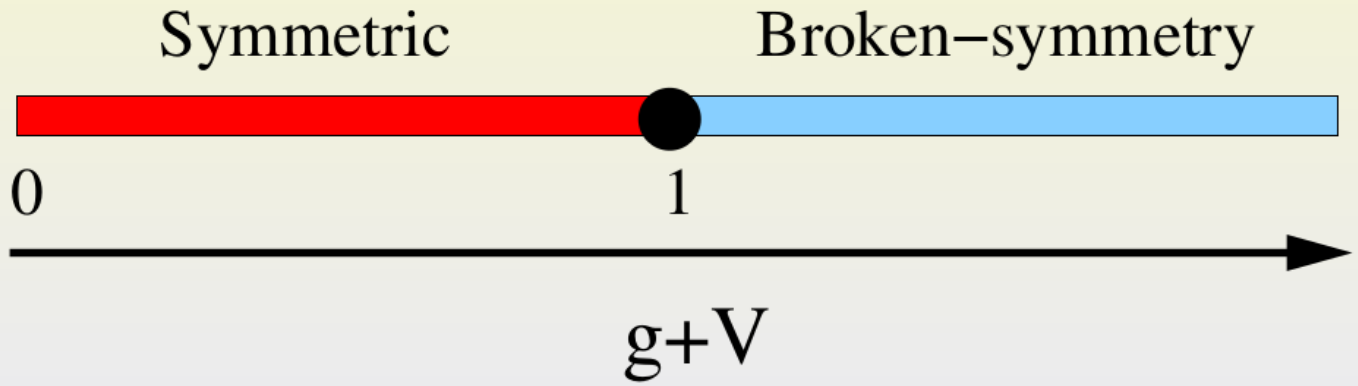
The Hamiltonian

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

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

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 $g + V > 1$



What do we measure?

The evolution operator

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

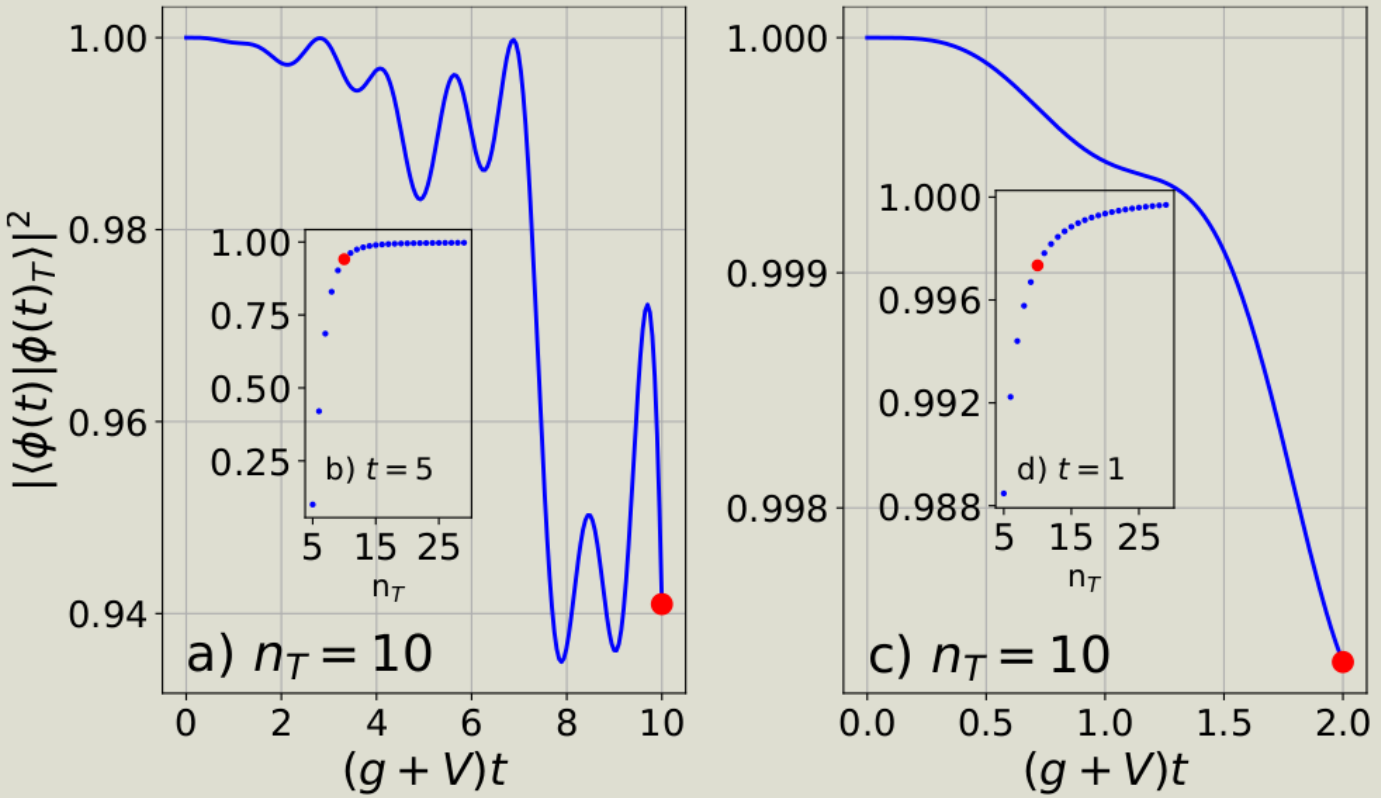
Experimentally it is implemented through the Lie-Trotter-Suzuki decomposition (Trotter in short)

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

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?

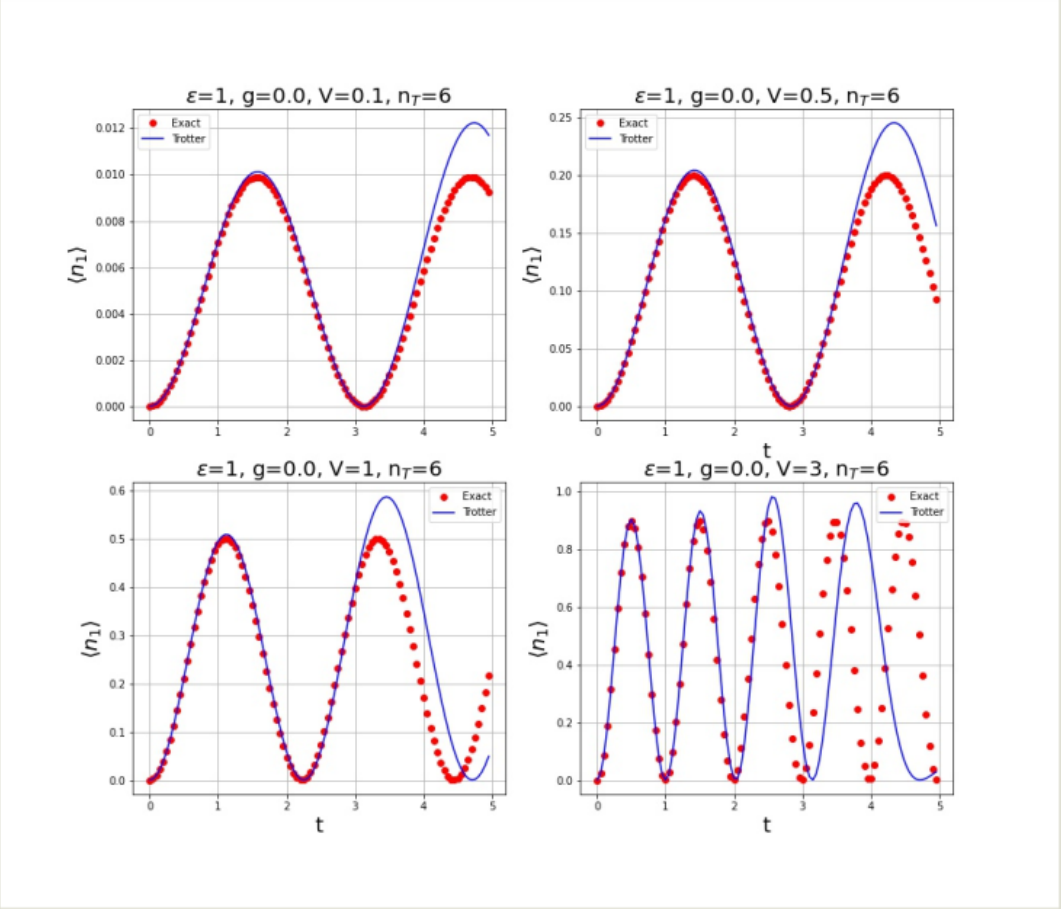
The fidelity



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 $g = V = 1$.

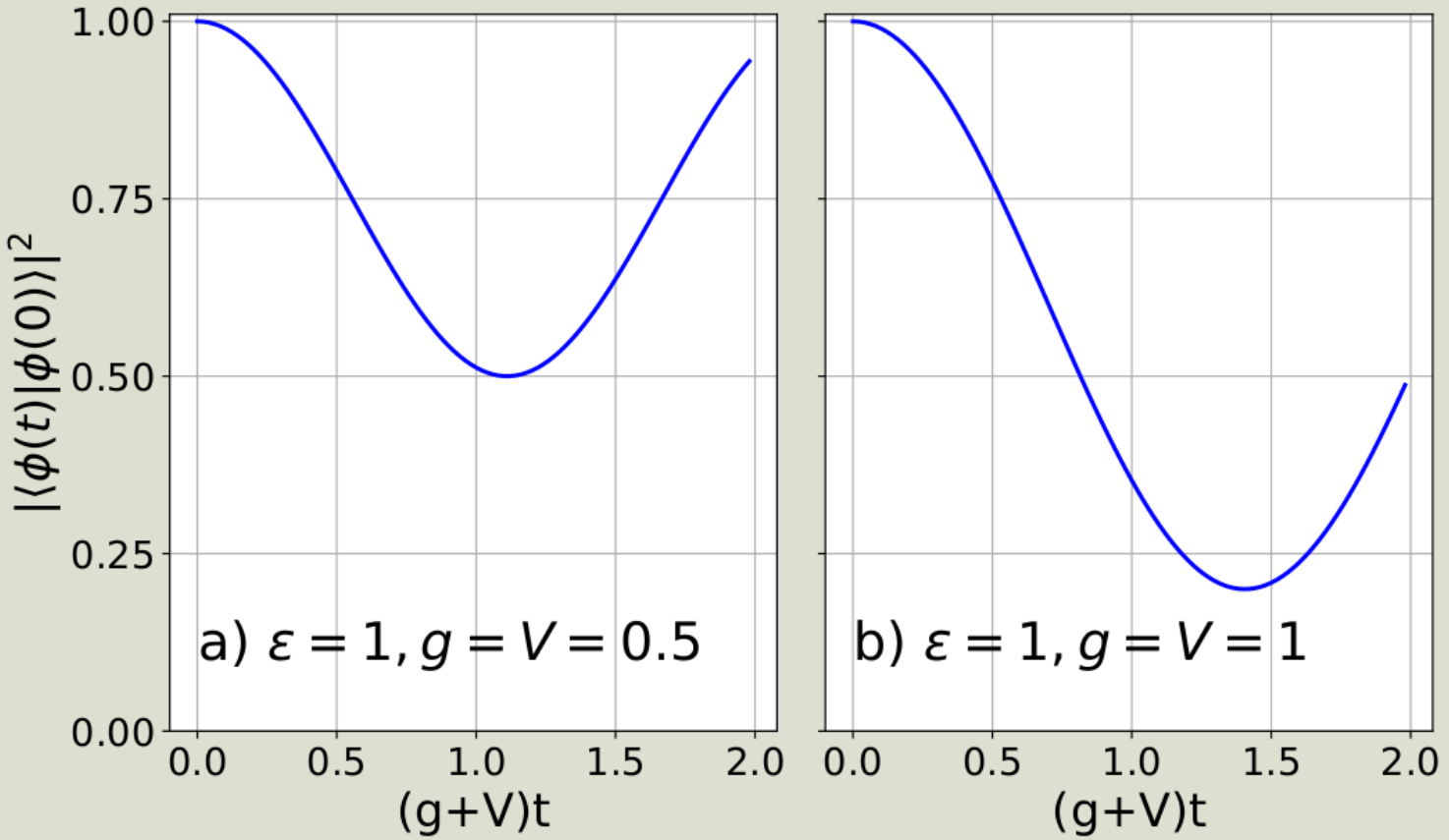
How good is the Trotter approach?

The value of $\langle n_1 \rangle$



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 survival probability



The initial state is $|\downarrow_1 \otimes \downarrow_2 \otimes \uparrow_3 \otimes \uparrow_4\rangle$ (with minimum value of $\langle J^0 \rangle = -1$).

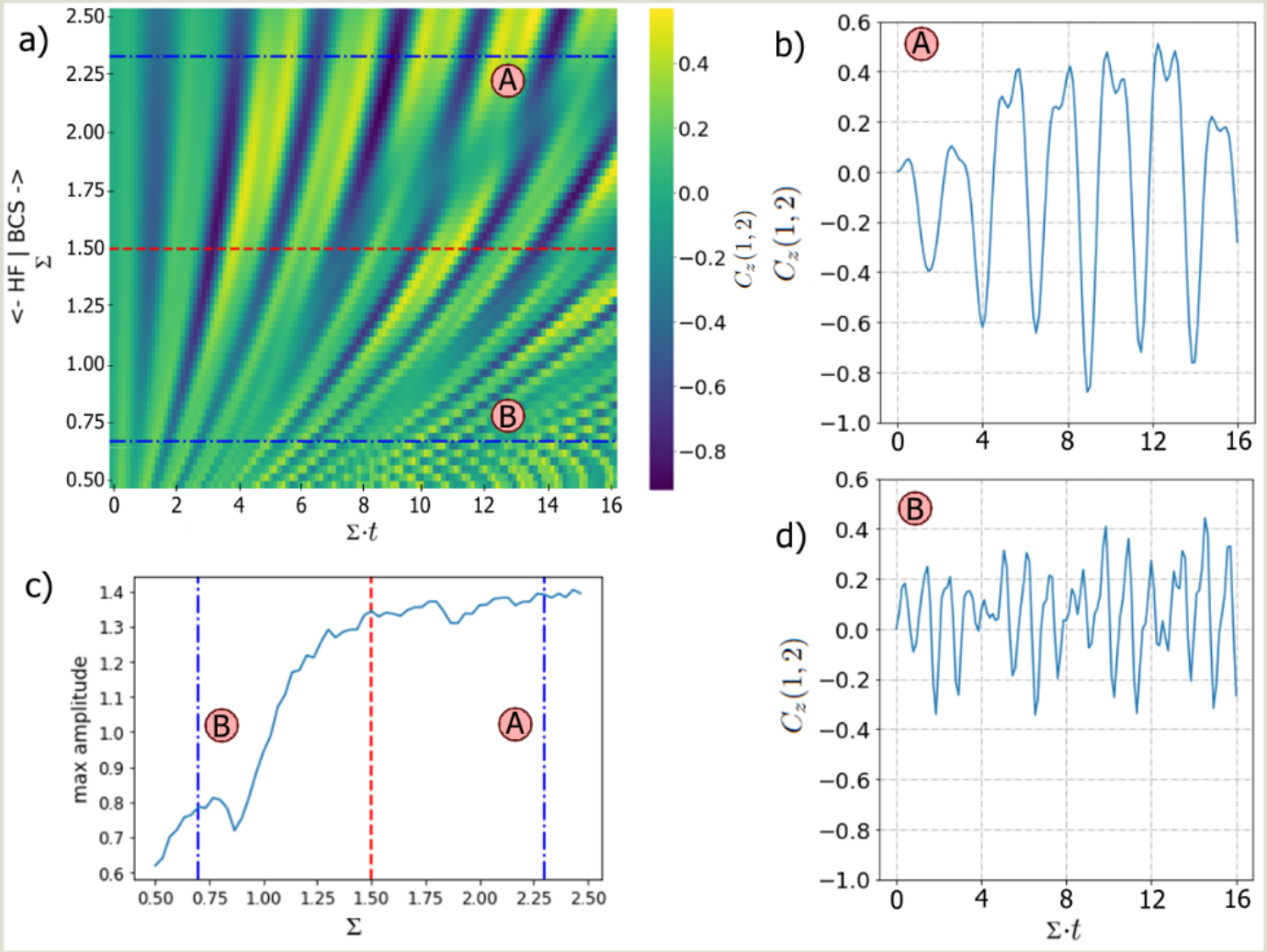
Feasibility

- $\exp(-iH_1 t)$: 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.

- 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%).

j=2, N=8 case

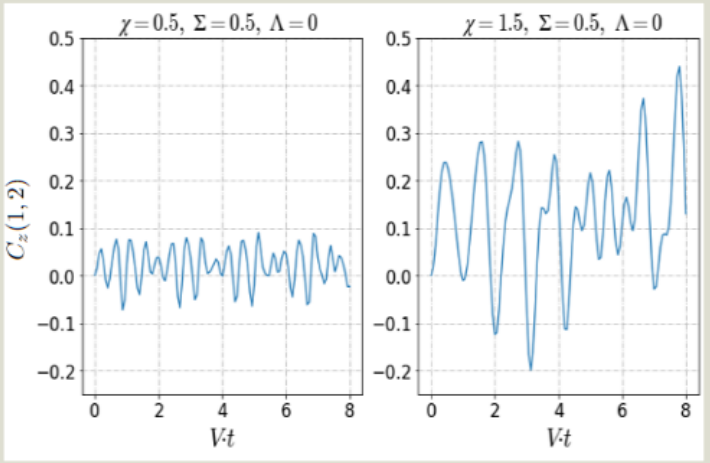
How to determine the phase in this case?



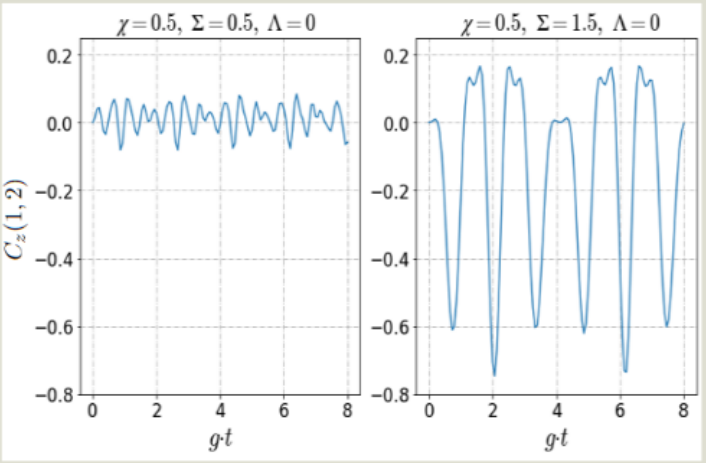
j=2, N=8 case

Different patterns everywhere

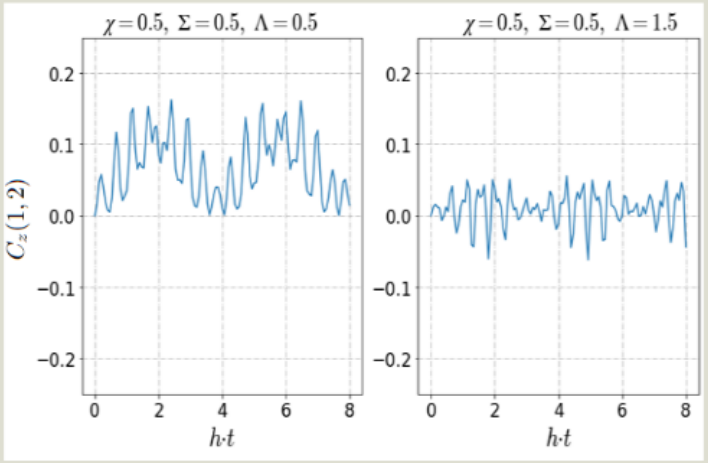
Symmetric HF



Symmetric BCS



Symmetric Combined



j=2, N=8 case

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.

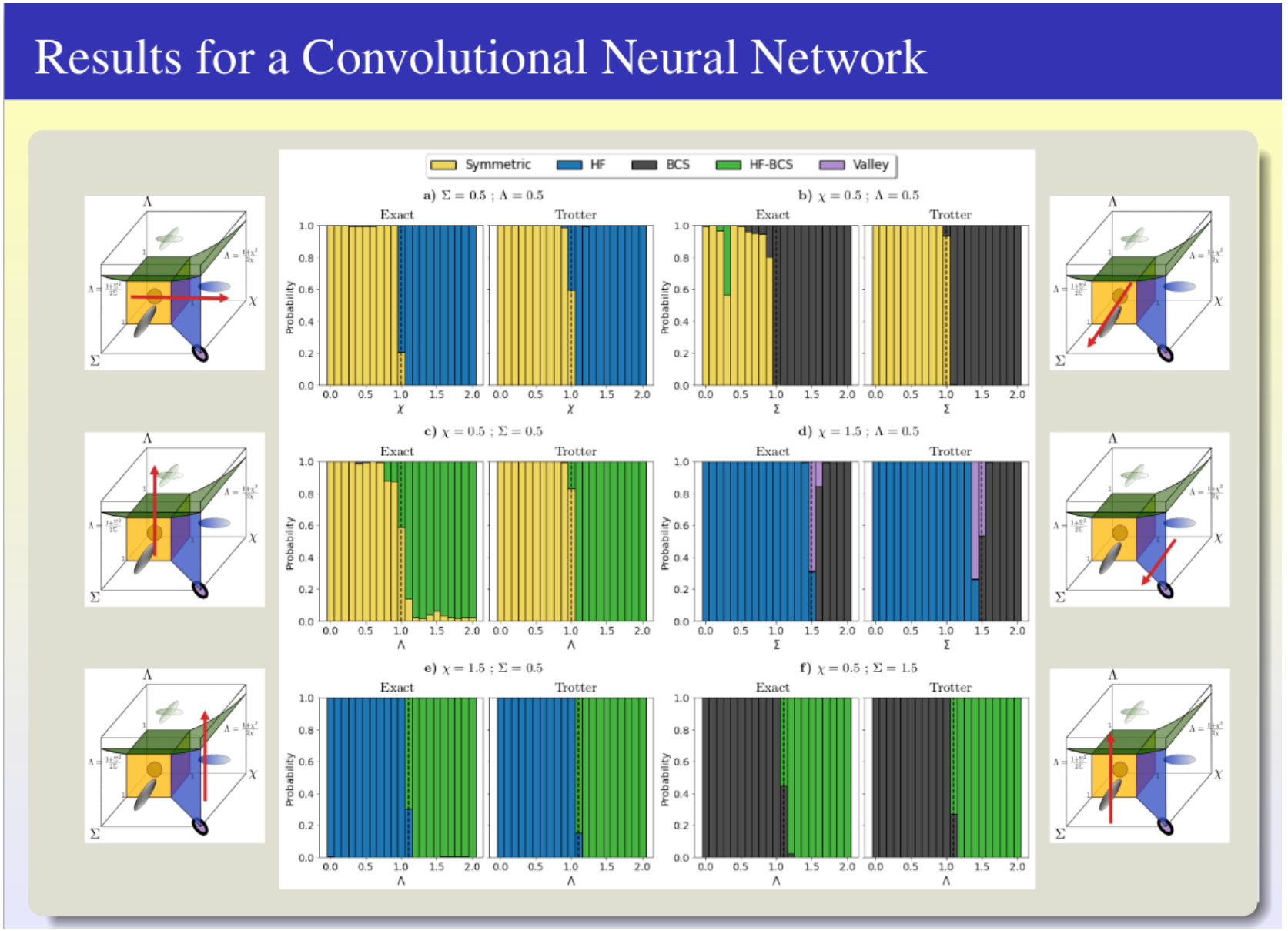
j=2, N=8 case

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.

j=2, N=8 case



Álvaro Saiz, Pedro Pérez-Fernández, José-Miguel Arias, José-Enrique García-Ramos, and Lucas Lamata, "Digital quantum simulation of an extended Agassi model: Using machine learning to disentangle its phase-diagram", **Phys, Rev. C 106, 064322 (2022).**

The ELM as an approximation of the Interacting Boson Model

The ELM Hamiltonian *à la* CQF

$$H = (1-\lambda)\, n_t - \frac{\lambda}{N}\, Q^{(\alpha)} \cdot Q^{(\alpha)},$$

$n_t = t^\dagger t$ and $Q^{(\alpha)} = (s^\dagger t + t^\dagger s) + \alpha(t^\dagger t)$

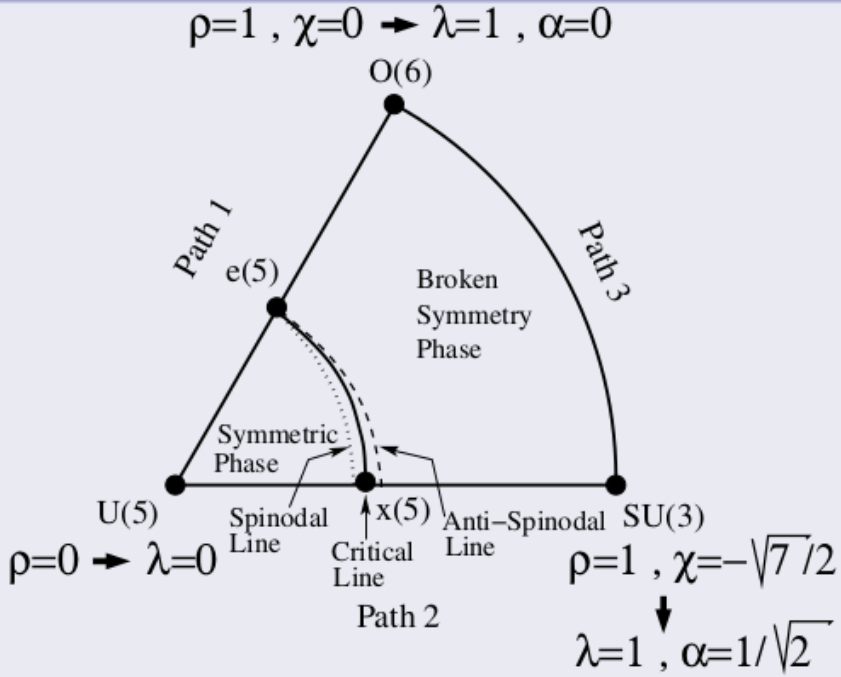
Equivalence with the Interacting Boson Model

$$S_+ = t^\dagger s$$

$$S_- = s^\dagger t,$$

$$S_z = \frac{1}{2}(t^\dagger t - s^\dagger s).$$

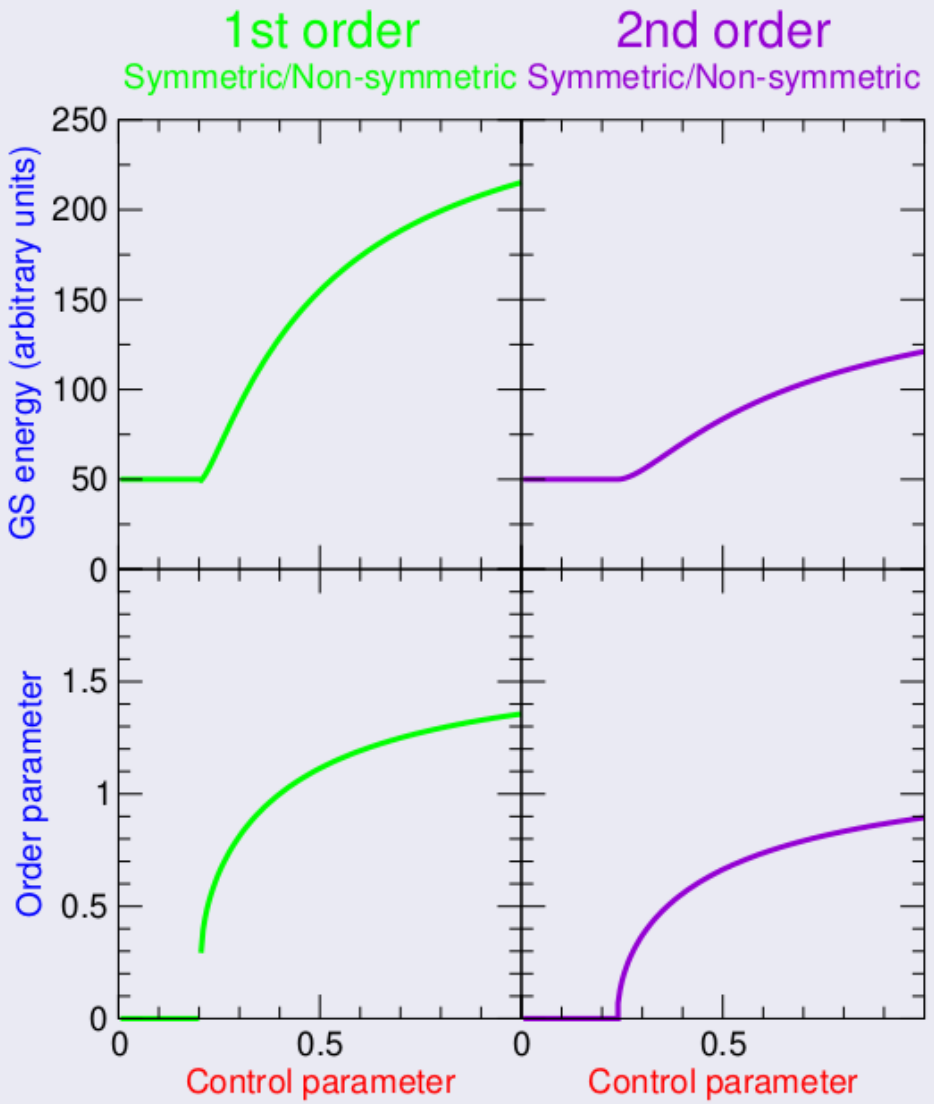
$$H_{EL} = H_L - \frac{\lambda}{N}\Big[\alpha^2(S+S_z)^2 - 2\alpha\big(S_x(S+S_z) + (S+S_z)S_x\big)\Big],$$



What a Quantum Phase Transition (QPT) is?

A QPT appears when the ground state a quantum system experiences a sudden change in its structure (order parameter) when a parameter that affects the Hamiltonian (control parameter) slightly changes around its critical value. This transitions are assumed to occurs at zero temperature.

$$\hat{H} = (1-\xi)\hat{H}_1 + \xi\hat{H}_2$$



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What Quantum Computing can do for Nuclear Physics?

J.E. García-Ramos

Departamento de Ciencias Integradas y
Centro de Estudios Avanzados en Física, Matemáticas y Computación,
Universidad de Huelva, Spain

FÍSICA MATEMÁTICAS COMPUTACIÓN

Universidad de Huelva

Supported by MCIN/ AEI/10.13039/501100011033
PID2022-136228NB-C21

Overview

- What is Quantum Computing?
  - Bits and Qubits. Gates and quantum gates
- First applications in Nuclear Physics
- Other selected applications
  - Shell model calculations
  - The phase diagram of the Agassi model
- Conclusions

What is Quantum Computing?

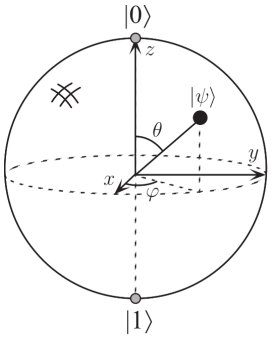
Bits and qubits

Bits: 0 or 1

Qubits:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$



Bloch sphere

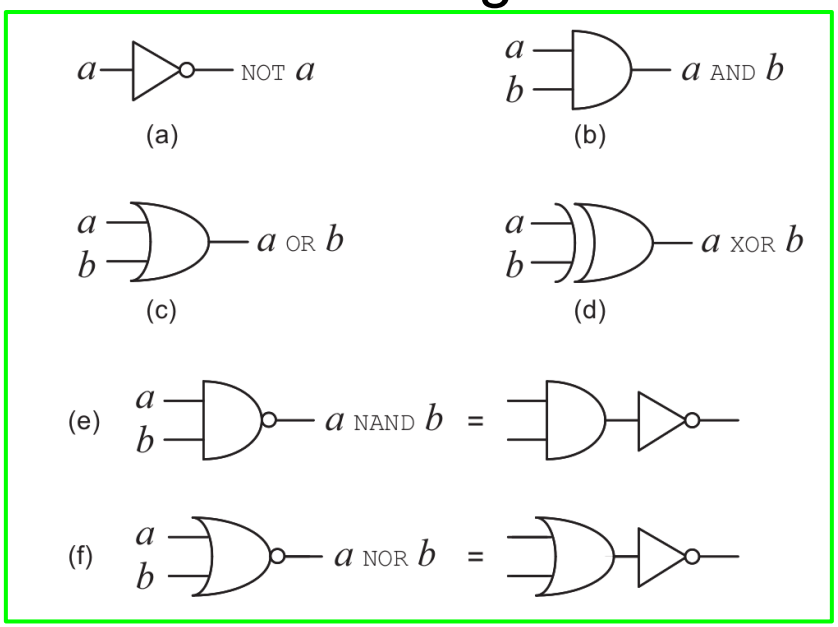
Multiple Qubits:

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

Bell state: $\dfrac{|00\rangle + |11\rangle}{\sqrt{2}}$

M. A. Nielsen, I. L. Chuang, Quantum Computation and Quantum Information

Classical gates



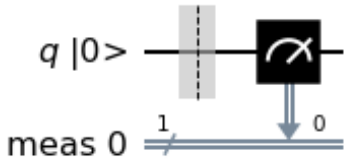
M. A. Nielsen, I. L. Chuang, Quantum Computation and Quantum Information

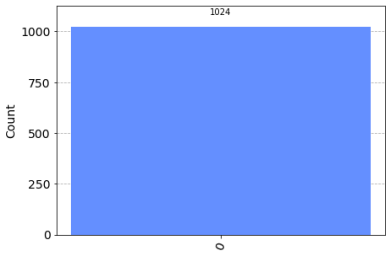
1 qubit quantum gates

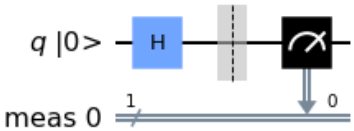
Hadamard	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Pauli-X	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Phase	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$

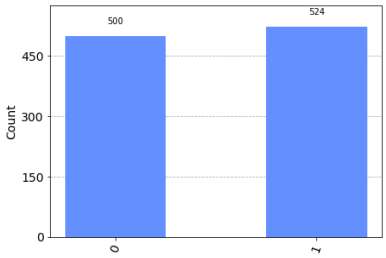
M. A. Nielsen, I. L. Chuang, Quantum Computation and Quantum Information

Some simple circuits









Results from qiskit Qiskit

Why Quantum Computing in Nuclear Physics

•The U.S. Department of Energy in its document Energy Research Opportunity II (2019) establishes “A broad theory program should be supported, which can, e.g., **develop methods to address problems in NP using digital quantum computers and quantum simulators**, **utilize QIS concepts** to better understand nuclear phenomena (such as the nuclear many-body problem andhadronization), and develop new QIS applications of importance to nuclear physics”.

•In the future, quantum computers will allow to outperform present computational (classical) capabilities.

•The applications of Quantum Computing in Nuclear Physics are increasing.

First applications in Nuclear Physics

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Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu, A. J. McCaskey, G. Hagen, G. R. Jansen, T. D. Morris, T. Papenbrock, R. C. Pooser, D. J. Dean, and P. Lougovski

Phys. Rev. Lett. 120, 210501 (2018)

- Quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers.
- Use of a variational wave-function ansatz based on unitary coupled-cluster theory (UCC)→ **Variational Quantum Eigensolver**

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n$$

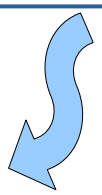
$$\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\Big[(2n+3/2)\delta^{n'}_n - \sqrt{n(n+1/2)}\delta^{n'+1}_n - \sqrt{(n+1)(n+3/2)}\delta^{n'-1}_n\Big],$$

$$V_0 = -5.68658111 \text{ MeV}$$

$$\hbar\omega = 7 \text{ MeV}$$

$$\langle n'|V|n\rangle = V_0\delta^0_n\delta^{n'}_n.$$

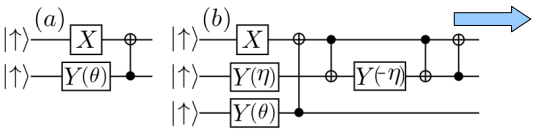
$$\begin{aligned} H_1 &= 0.218291(Z_0 - I) \\ H_2 &= 5.906709I + 0.218291Z_0 - 6.125Z_1 \\ &\quad - 2.143304\,(X_0X_1 + Y_0Y_1)\,, \\ H_3 &= H_2 + 9.625(I - Z_2) \\ &\quad - 3.913119\,(X_1X_2 + Y_1Y_2)\,. \end{aligned}$$



Jordan-Wigner transformation

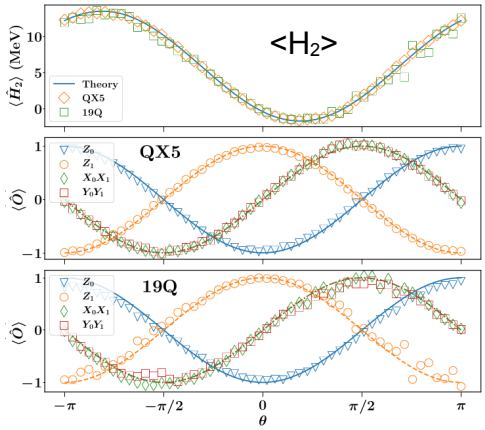
Cloud Quantum Computing of an Atomic Nucleus

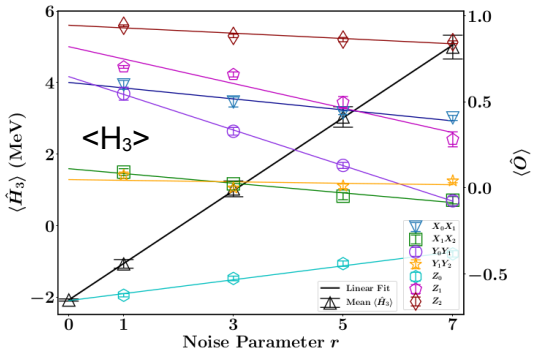
Variational wave function



$$U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)},$$

$$U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)+\theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$
$$\approx e^{i\frac{\eta}{2}(X_0Y_1 - X_1Y_0)} e^{i\frac{\theta}{2}(X_0Z_1Y_2 - X_2Z_1Y_0)}$$





E(exact)=-2.22 MeV, E(H_2)=-2.18 MeV, E(H_3)=-2.21MeV

The Jordan-Wigner transformation

The transformation

$$c_i^\dagger = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^- \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$
$$c_i = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^+ \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$

with

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

and

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

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The Variational Quantum Eigensolver (VQE)

nature COMMUNICATIONS

ARTICLE

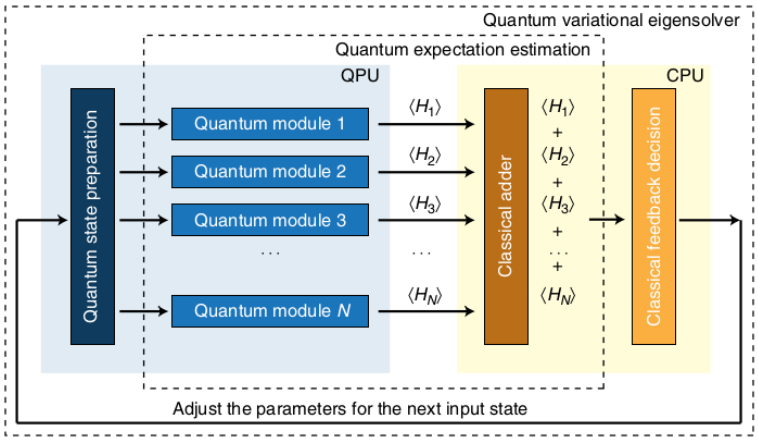
Received 9 Dec 2013 | Accepted 27 May 2014 | Published 23 Jul 2014 DOI: 10.1038/ncomms5213 OPEN

A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo[1,*†], Jarrod McClean[2,*], Peter Shadbolt[1], Man-Hong Yung[2,3], Xiao-Qi Zhou[1], Peter J. Love[4], Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]

$$E_0 \leqslant \frac{\langle\psi|\,\hat{H}\,|\psi\rangle}{\langle\psi|\psi\rangle}. \qquad E_{\mathrm{VQE}} = \min_{\theta} \langle \mathbf{0}|\, U^{\dagger}(\theta)\hat{H}U(\theta)\,|\mathbf{0}\rangle .$$

$$\hat{H} = \sum_{a}^{\mathcal{P}} w_a \hat{P}_a, \qquad E_{\mathrm{VQE}} = \min_{\theta} \sum_{a}^{\mathcal{P}} w_a \langle \mathbf{0}|\, U^{\dagger}(\theta)\hat{P}_a U(\theta)\,|\mathbf{0}\rangle ,$$



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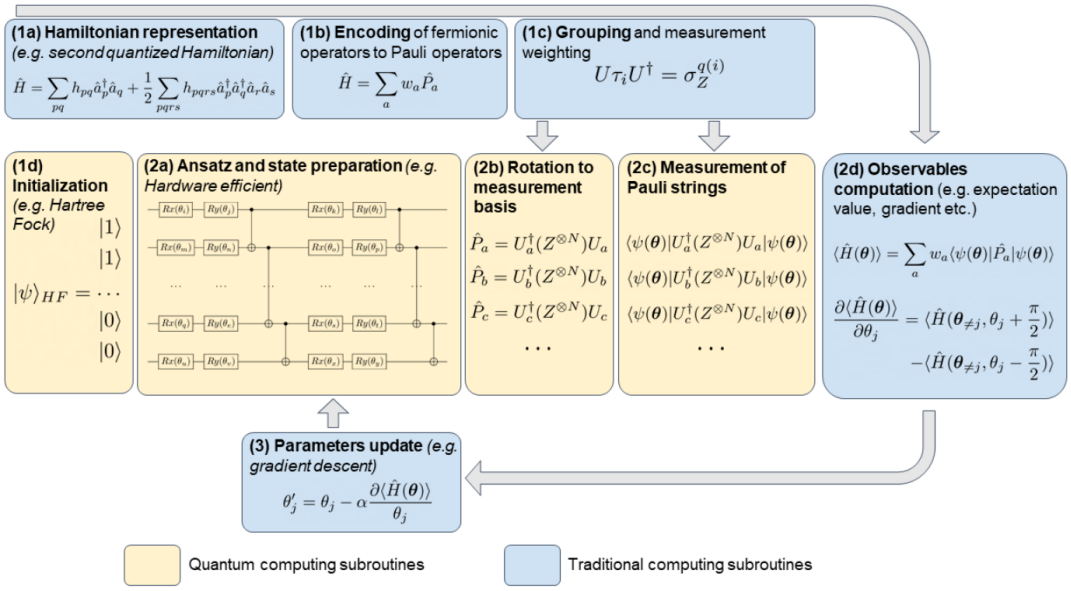
The Variational Quantum Eigensolver (VQE)



J. Tilly, et al, "The Variational Quantum Eigensolver: A review of methods and best practices", Physics Reports 986, 1 (2022).

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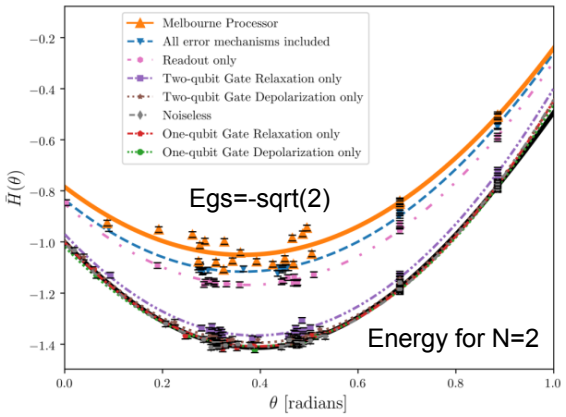
Lipkin model on a quantum computer

M. J. Cervia, A. B. Balantekin, S. N. Coppersmith, Calvin W. Johnson, Peter J. Love, C. Poole. K. Robbins, and M. Saffman
Physical Review C 104, 024305 (2021)

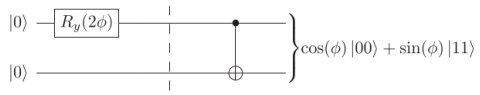
•Quantum simulation of the Lipkin Hamiltonian binding energy on quantum processors accessed via cloud servers.
•Use of a variational wave-function ansatz → **VQE**
•No Jordan-Wigner transformation is needed.

$$H = \sum_{p=1}^{N} J_0^{(p)} + V \sum_{\substack{p,q=1 \\ q \neq p}}^{N} (J_+^{(p)} J_+^{(q)} + J_-^{(q)} J_-^{(p)}).$$

Results for N=**2**, 3, 4

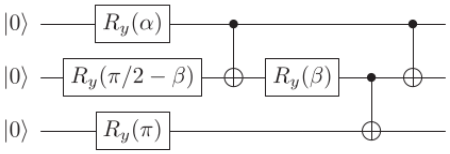


Trial wave function for N=2



$\cos(\phi)\,|00\rangle + \sin(\phi)\,|01\rangle$

Trial wave function for N=3



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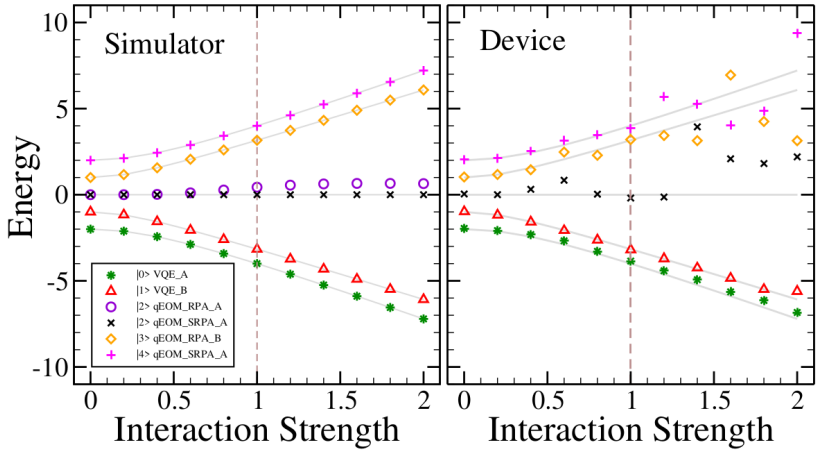
Simulating excited states of the Lipkin model on a quantum computer

Manqoba Q. Hlatshwayo, Yinu Zhang, Herlik Wibowo, Ryan LaRose, Denis Lacroix, and Elena Litvinova

Phys. Rev. C 106, 024319 (2022)

- Quantum simulation of the excited state energies for the Lipkin model.
- Use of the Quantum Equation of Motion (qEOM) method.
- Calculations for N = 2, 3 and 4 particles.
- The accuracy strongly depend on the fermion to qubit encoding.



N=4

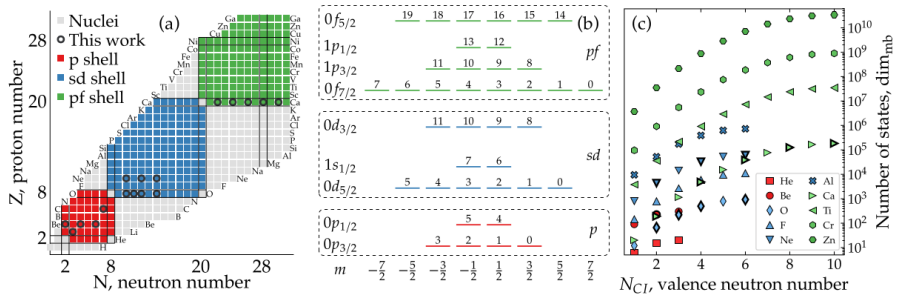
Other selected applications: Shell Model calculations

Nuclear shell-model simulation in digital quantum computers

A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz

Scientific Reports 13:12291 (2023)

- Use of the adaptive variational quantum eigensolver algorithm (ADAPT-VQE).
- Calculation of the ground state energy in the p, sd, and pf shells.



Shell	N_{qb}	N_h	N_{hh}	N_{tot}
p	6	2	10 (9)	13 (12)
	12	4	109 (44)	114 (49)
sd	12	8	203 (86)	212 (95)
	24	16	1389 (518)	1406 (535)
pf	20	20	1507 (570)	1528 (591)
	40	40	10,572 (3459)	10,613 (3500)

Number of circuits

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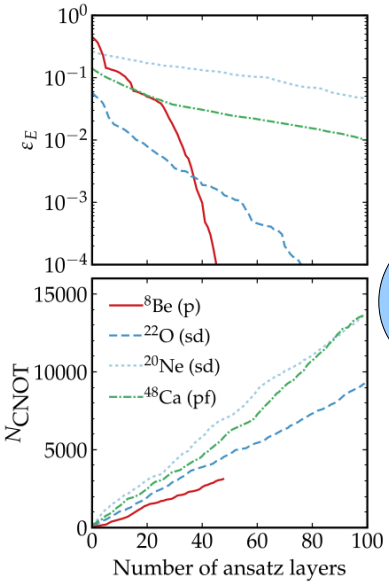
Nuclear shell-model simulation in digital quantum computers

A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz

Scientific Reports 13:12291 (2023)

Accuracy and number of CNOTs



ADAPT-VQE method

$$|\psi(\boldsymbol{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k} |\mathrm{ref}\rangle \qquad |\psi(\boldsymbol{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k} |\mathrm{ref}\rangle$$

$$\left.\frac{\partial E^{(n)}}{\partial \theta_k}\right|_{\theta_k=0} = i\langle\psi(\boldsymbol{\theta})|[H_{\mathrm{eff}}, A_k]|\psi(\boldsymbol{\theta})\rangle|_{\theta_k=0}$$

The new operator is selected according to the largest energy gradient

Pool of operators: $T_{rs}^{pq} = i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$

Nuclear shell-model simulation in digital quantum computers

A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz

Scientific Reports 13:12291 (2023)

	Fermion operators	Qubit operators
n_p	$a_p^\dagger a_p$	$\frac{1}{2}(1 - Z_p)$
h_{pqrs}	$a_p^\dagger a_q^\dagger a_r a_s$ $+a_r^\dagger a_s^\dagger a_p a_q$	$\frac{1}{8} P_{rs}^{pq} (-X_p X_q X_r X_s + X_p X_q Y_r Y_s$ $-X_p Y_q X_r Y_s - X_p Y_q Y_r X_s$ $-Y_p Y_q Y_r Y_s + Y_p Y_q X_r X_s$ $-Y_p X_q Y_r X_s - Y_p X_q X_r Y_s)$
T_{rs}^{pq}	$i(a_p^\dagger a_q^\dagger a_r a_s$ $-a_r^\dagger a_s^\dagger a_p a_q)$	$\frac{1}{8} P_{rs}^{pq} (-X_p Y_q Y_r Y_s - Y_p X_q Y_r Y_s$ $+Y_p Y_q X_r Y_s + Y_p Y_q Y_r X_s$ $+Y_p X_q X_r X_s + X_p Y_q X_r X_s$ $-X_p X_q Y_r X_s - X_p X_q X_r Y_s)$
h_{pq}	$a_p^\dagger a_q + a_q^\dagger a_p$	$\frac{1}{2}\left(\prod_{n=p+1}^{q-1} Z_n\right)(X_p X_q + Y_q Y_p)$
T_{pq}	$i(a_p^\dagger a_q - a_q^\dagger a_p)$	$\frac{1}{2}\left(\prod_{n=p+1}^{q-1} Z_n\right)(Y_p X_q - X_q Y_p)$

$$a_i^\dagger = \left(\prod_{k=0}^{i-1} Z_k\right)\sigma_i^-, \quad a_i = \left(\prod_{k=0}^{i-1} Z_k\right)\sigma_i^+$$

$$P_{rs}^{pq} \equiv \left(\prod_{m=p+1, m\notin[r,s]}^{q-1} Z_m\right)\left(\prod_{n=r+1, n\notin[p,q]}^{s-1} Z_n\right)$$

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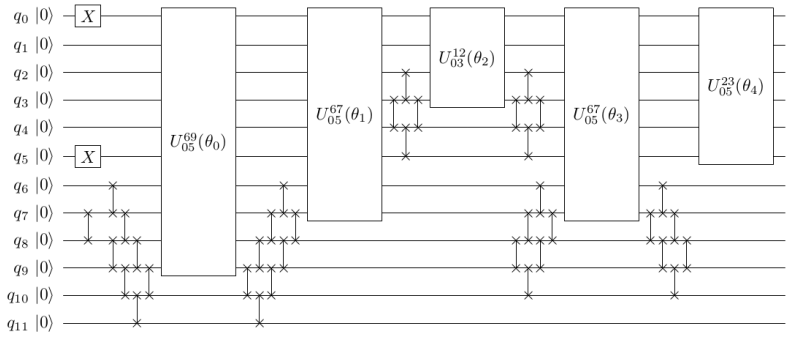
A. Pérez-Obiol, A. M. Romero, J. Menéndez, A. Rios, A. García-Sáez, and B. Juliá-Díaz

Scientific Reports 13:12291 (2023)

Circuit for ^{18}O



The measurements

$$\langle\psi_n|n_i|\psi_n\rangle = \frac{1}{2}\langle\psi_n|1 - Z_i|\psi_n\rangle = p_1^{(i)} \qquad \langle\psi_n|h_{ijij}|\psi_n\rangle = -2\langle\psi_n|n_i n_j|\psi_n\rangle = -2p_{11}^{(ij)}$$

$$\langle\psi_n|h_{ijik}|\psi_n\rangle = p_{101}^{(ijk)} - p_{110}^{(ijk)} \qquad \langle\psi_n|h_{ijik}|\psi_n\rangle = p_{101}^{(ijk)} - p_{110}^{(ijk)}$$

Other selected applications: Phase diagram of the Agassi model

A digital quantum simulation of the Agassi model,
P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

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).

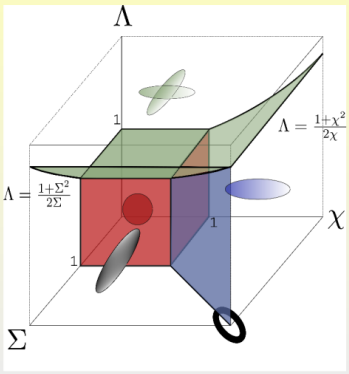
The original Hamiltonian

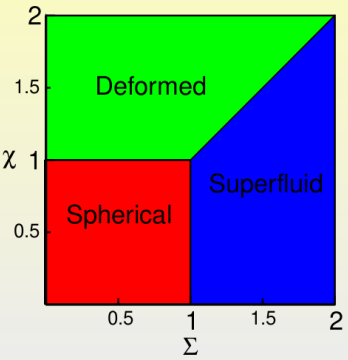
$$H = \frac{1}{2}\epsilon\sum_{m\sigma}\sigma a^\dagger_{m\sigma}a_{m\sigma} + \frac{1}{2}V\sum_{mm'\sigma} a^\dagger_{m\sigma}a^\dagger_{m'\sigma}a_{m'-\sigma}a_{m-\sigma} - \frac{1}{4}g\sum_{mm'\sigma\sigma'} a^\dagger_{m\sigma}a^\dagger_{-m\sigma}a_{-m'-\sigma'}a_{m'\sigma'}$$

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

A digital quantum simulation of the Agassi model,
P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

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))

A digital quantum simulation of the Agassi model,
P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

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.

A different view

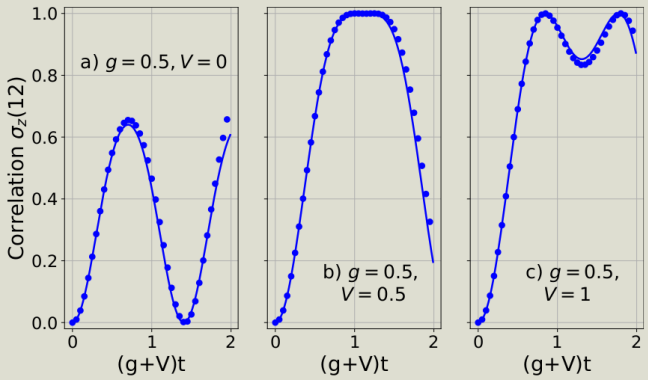
- The shape of the system characterizes its spectrum.
- An observable depending on the spectrum could encode the shape of the system. That, in general, will happen for the time evolution of the matrix element of a non-eigenstate.
- Most probably the results will depend on the state and on the used operator.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

A digital quantum simulation of the Agassi model,
P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

Is it possible to determine the phase of the system?

The correlation function

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

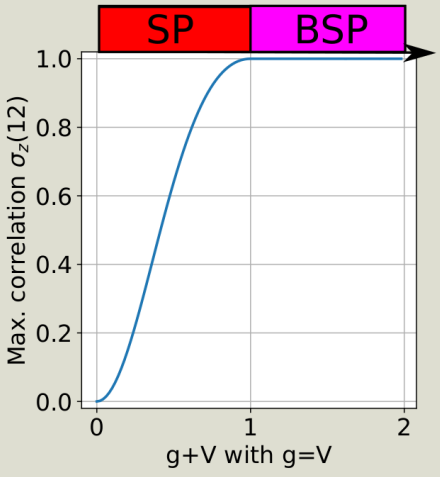


The initial state is $|\downarrow_1 \otimes \downarrow_2 \otimes \uparrow_3 \otimes \uparrow_4\rangle$ (exact and Trotter results).

A digital quantum simulation of the Agassi model,
P. Pérez-Fernández, J.M. Arias, J.E. García-Ramos, and L. Lamata,
Physics Letters B 829, 137133 (2022).

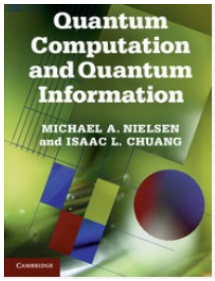
Is it possible to determine the phase of the system?

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



Still interested?
Really willing to start with QC?

To start with



PHYSICAL REVIEW A, VOLUME 65, 042323

Simulating physical phenomena by quantum networks

R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme
Los Alamos National Laboratory, Los Alamos, New Mexico 87545
(Received 12 September 2001; published 9 April 2002)

Physical systems, characterized by an ensemble of interacting constituents, can be represented and studied by different algebras of operators (observables). For example, a fully polarized electronic system can be studied by means of the algebra generated by the usual fermionic creation and annihilation operators or by the algebra of Pauli (spin-1/2) operators. The Jordan-Wigner isomorphism gives the correspondence between the two algebras. As we previously noted, similar isomorphisms enable one to represent any physical system in a quantum computer. In this paper we evolve and exploit this fundamental observation to simulate generic physical phenomena by quantum networks. We give quantum circuits useful for the efficient evaluation of the physical properties (e.g., the spectrum of observables or relevant correlation functions) of an arbitrary system with Hamiltonian H.

Interested in doing calculations?

Qiskit https://qiskit.org/, https://quantum.ibm.com/

Cirq https://quantumai.google/cirq

OpenFermion https://quantumai.google/openfermion

Universidad de Huelva
www.uhu.es/fmc

(Personal) Conclusions

- Quantum Computing in Nuclear Physics is still in its infancy, specially if compared with Molecular Physics.
- The calculations that can be afforded today can be easily done in a standard HPC cluster, if not in a laptop.
- There is a lot of room for the implementation and design of new algorithms in Quantum Computing.
- The use of Quantum Computing and Quantum Information techniques can strongly contribute to the development of new “classical” Nuclear Structure ideas.

Thank you

2 qubits quantum gates

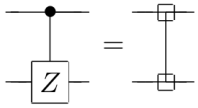
controlled-NOT

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

swap

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

controlled-Z



$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

controlled-phase

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}$$

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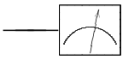
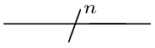
Other elements

measurement		Projection onto $\|0\rangle$ and $\|1\rangle$
qubit		wire carrying a single qubit (time goes left to right)
classical bit		wire carrying a single classical bit
n qubits		wire carrying n qubits

$$R_x(\theta) \equiv e^{-i\theta X/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} X = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_y(\theta) \equiv e^{-i\theta Y/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} Y = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

$$R_z(\theta) \equiv e^{-i\theta Z/2} = \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2} Z = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix}.$$

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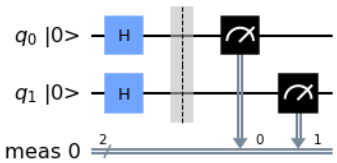
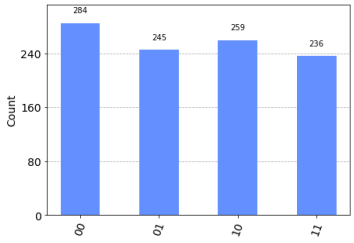
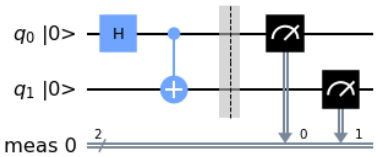
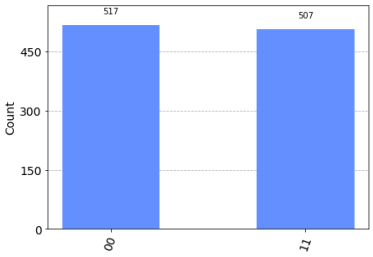
A step further







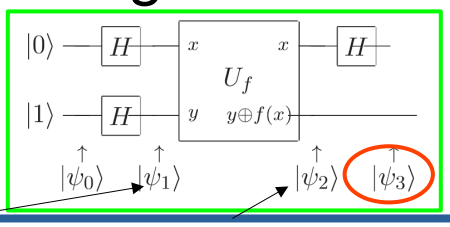


Results from qiskit Qiskit

Deutsch's algorithm

Let us a function, f: {0,1} → {0,1}

Problem: to calculate whether
f(0)=f(1) or f(0)≠f(1)



$$|\psi_1\rangle = \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

$$|\psi_2\rangle = \begin{cases} \pm\left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) = f(1) \\ \pm\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) \neq f(1). \end{cases}$$

$$(-1)^{f(x)}|x\rangle(|0\rangle - |1\rangle)/\sqrt{2}$$

$$|\psi_3\rangle = \begin{cases} \pm|0\rangle\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) = f(1) \\ \pm|1\rangle\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] & \text{if } f(0) \neq f(1). \end{cases}$$

$$|\psi_3\rangle = \pm|f(0) \oplus f(1)\rangle\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

With a single measurement we solve the problem,
while classically we need two measurements!!
|q0> = |0> → **f(0)=f(1)**
|q1> = |1> → **f(0)≠f(1)**

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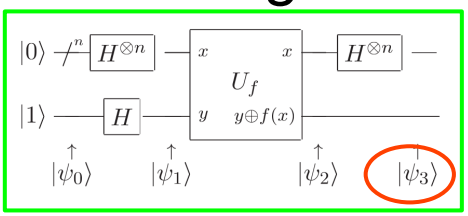
The Deutsch–Jozsa algorithm

Let us a function, f: [0,2^n-1] → {0,1}
Problem: is it the function perfectly balanced or is it constant?



$$|0\rangle^{\otimes n}|1\rangle$$

$$|\psi_1\rangle = \sum_{x\in\{0,1\}^n} \frac{|x\rangle}{\sqrt{2^n}} \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

$$|\psi_2\rangle = \sum_x \frac{(-1)^{f(x)}|x\rangle}{\sqrt{2^n}} \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

$$H^{\otimes n}|x_1,\ldots,x_n\rangle = \frac{\sum_{z_1,\ldots,z_n}(-1)^{x_1z_1+\cdots+x_nz_n}|z_1,\ldots,z_n\rangle}{\sqrt{2^n}} \qquad H^{\otimes n}|x\rangle = \frac{\sum_z(-1)^{x\cdot z}|z\rangle}{\sqrt{2^n}}$$

$$|\psi_3\rangle = \sum_z \sum_x \frac{(-1)^{x\cdot z+f(x)}|z\rangle}{2^n} \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$

For f constant: probability of measuring $|0\rangle^{\otimes n}$ is one
For f balanced: probability of measuring $|0\rangle^{\otimes n}$ is zero
With a single measurement we solve the problem, while classically we need two $2^n/2+1$ measurements!!

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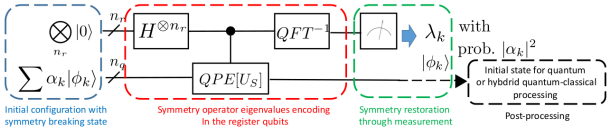
Symmetry-Assisted Preparation of Entangled Many-Body States on a Quantum Computer

Denis Lacroix

Phys. Rev. Lett. 125, 230502 (2020)

- Use of the Quantum Phase Estimation (QPE) algorithm, to construct entangled states that describe correlated many-body systems on quantum computers
- The QPE approach is followed by measurements that serve as projectors on the entangled states.
- The approach can be seen as a quantum–computer formulation of symmetry breaking followed by symmetry restoration.

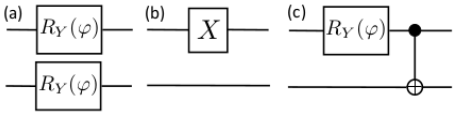


$$H_{\rm P} = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) - g \sum_{i,j>0} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j.$$

$$E/g = -\frac{1}{4}(A-\nu)(2n_q - A - \nu - 2)$$

$$|\psi\rangle = \prod_{n>0} e^{i\varphi(X_n Y_{n+1} + Y_n X_{n+1})/2} |-\rangle \quad \Rightarrow \quad |\psi\rangle = \prod_n \left[\cos\left(\frac{\varphi}{2}\right) I_n \otimes I_{n+1} + \sin\left(\frac{\varphi}{2}\right) Q_n^+ Q_{n+1}^+\right] |-\rangle$$

This state is obtained by applying this circuit to all (n, n + 1) pairs.



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Denis Lacroix
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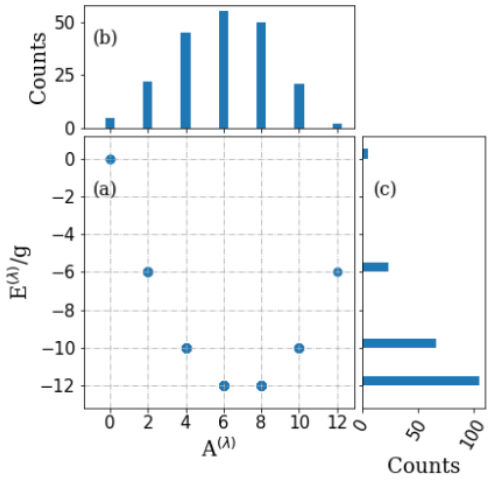
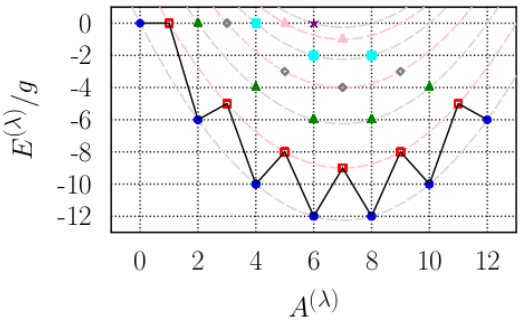




Complete spectrum obtained for n = 12

Correlation between the energies and the particle number. The distribution of counts for the particle number and energies are shown respectively in panels (b) and (c).

Agassi model

The O(5) as the spectrum generator algebra

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

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

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

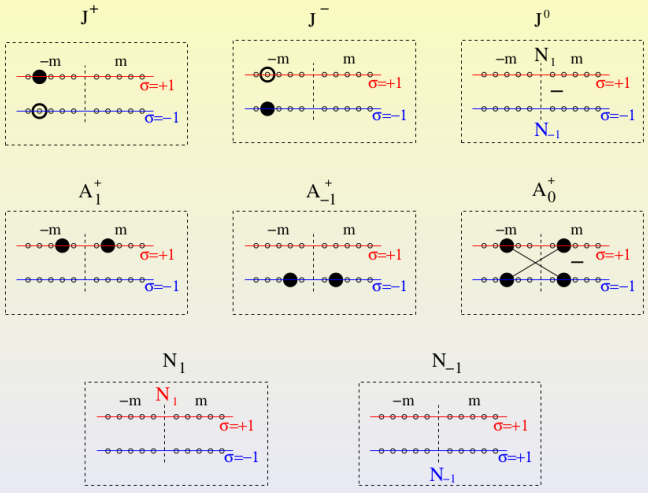
The Hamiltonian

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

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



Numerical calculations

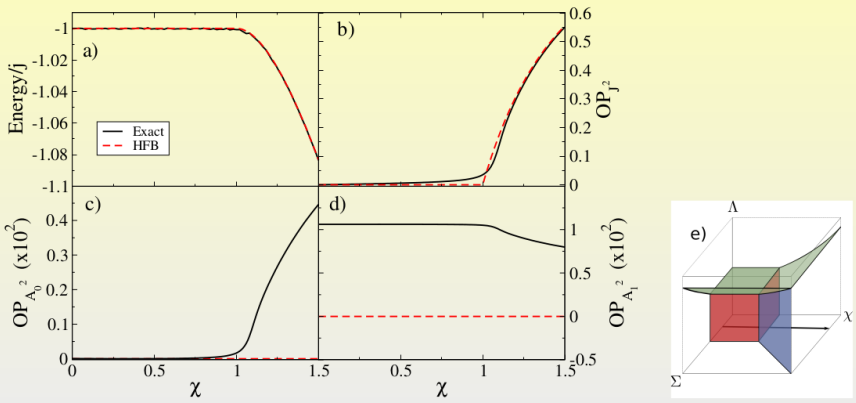


Figure: Comparison of HFB and exact results. $j = 100$ and Hamiltonian parameters $\Sigma = 0.5, \Lambda = 0$.

Numerical calculations

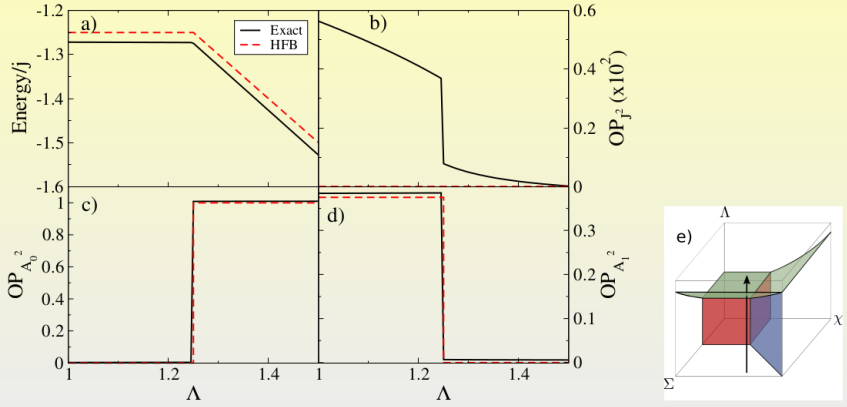


Figure: Comparison of HFB and exact results. $j = 100$ and Hamiltonian parameters $\chi = 1.5$, $\Sigma = 2$.

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

$$c_i^\dagger = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^- \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$
$$c_i = (-1)^{i-1} I_N \otimes \ldots \otimes I_{i+1} \otimes \sigma_i^+ \otimes \sigma_{i-1}^z \otimes \ldots \otimes \sigma_1^z ,$$

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

$$
\begin{aligned}
c_{1,1} &\rightarrow c_1, \\
c_{1,-1} &\rightarrow c_2, \\
c_{-1,1} &\rightarrow c_3, \\
c_{-1,-1} &\rightarrow c_4.
\end{aligned}
\qquad
\begin{aligned}
J^+ &= -\sigma_2^+ \otimes \sigma_3^z \otimes \sigma_4^- - \sigma_1^+ \otimes \sigma_2^z \otimes \sigma_3^-, \\
J^0 &= (1/4)(\sigma_1^z + \sigma_2^z - \sigma_3^z - \sigma_4^z), \\
J^- = (J^+)^\dagger &= -\sigma_2^- \otimes \sigma_3^z \otimes \sigma_4^+ - \sigma_1^- \otimes \sigma_2^z \otimes \sigma_3^+, \\
A_1^\dagger &= \sigma_1^+ \otimes \sigma_2^+, \; A_{-1}^\dagger = \sigma_3^+ \otimes \sigma_4^+, \\
A_1 &= \sigma_1^- \otimes \sigma_2^-, \; A_{-1} = \sigma_3^- \otimes \sigma_4^-.
\end{aligned}
$$

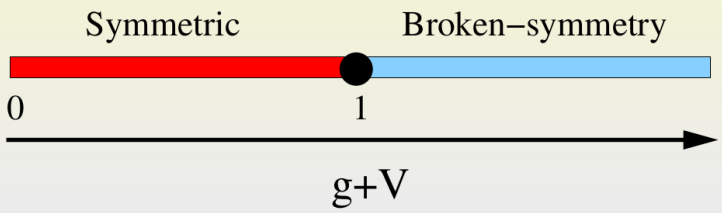
The Hamiltonian

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

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

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 $g + V > 1$



What do we measure?

The evolution operator

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

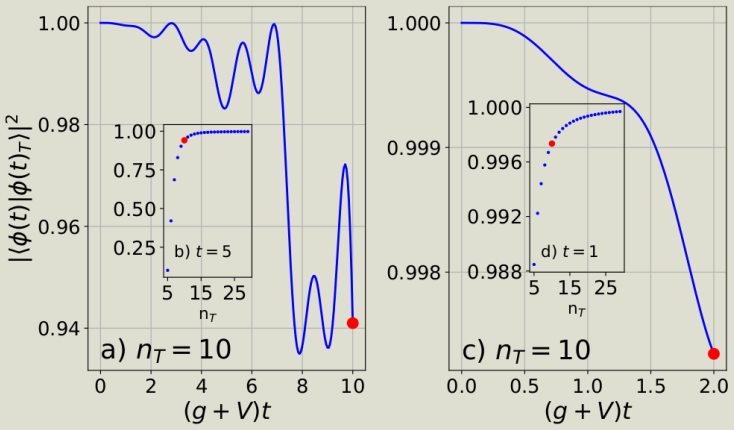
Experimentally it is implemented through the Lie-Trotter-Suzuki decomposition (Trotter in short)

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

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?

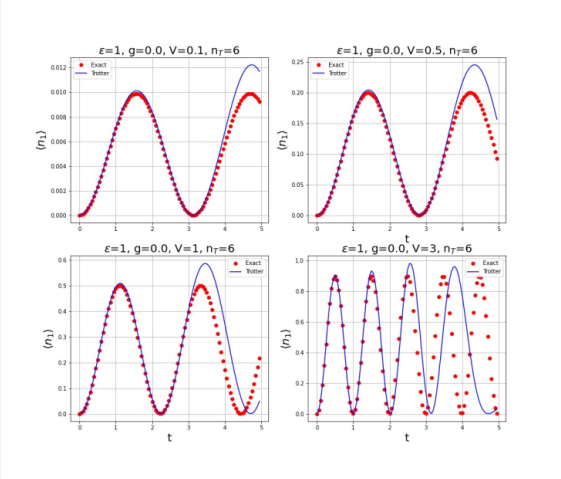
The fidelity



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 $g = V = 1$.

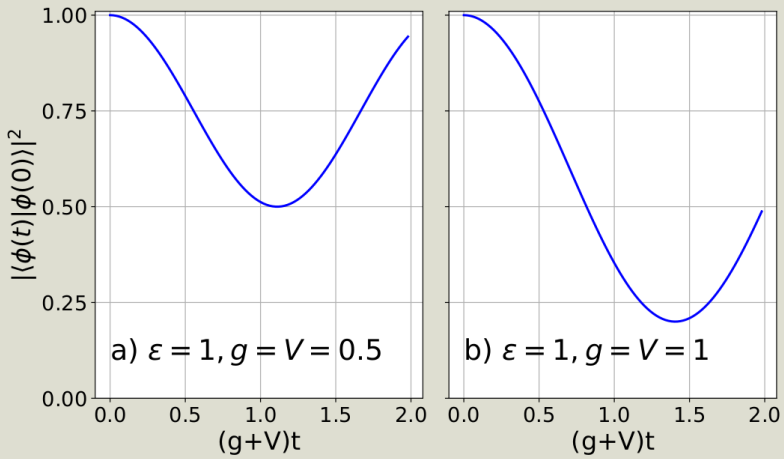
How good is the Trotter approach?

The value of $\langle n_1 \rangle$



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 survival probability



The initial state is $|\downarrow_1 \otimes \downarrow_2 \otimes \uparrow_3 \otimes \uparrow_4\rangle$ (with minimum value of $\langle J^0 \rangle = -1$).

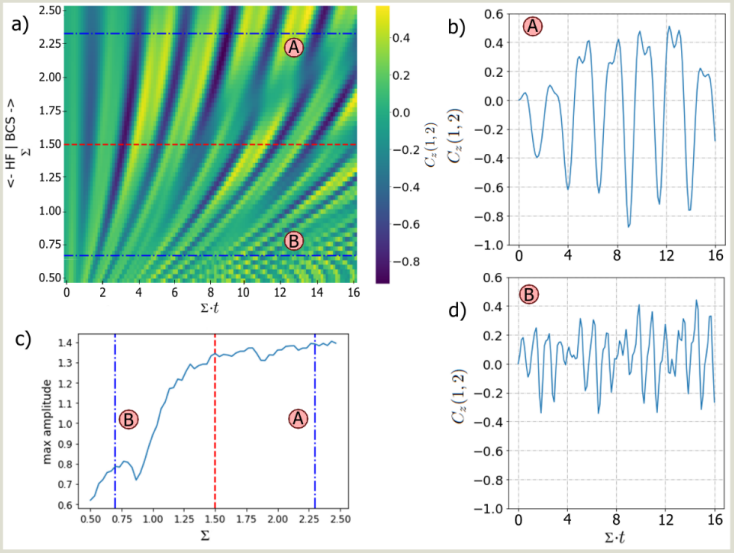
Feasibility

- $\exp(-iH_1 t)$: 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.

- 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%).

j=2, N=8 case

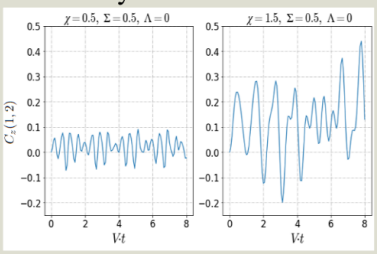
How to determine the phase in this case?



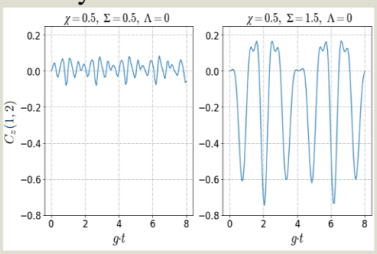
j=2, N=8 case

Different patterns everywhere

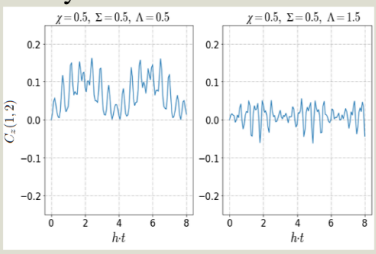
Symmetric HF



Symmetric BCS



Symmetric Combined



j=2, N=8 case

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.

j=2, N=8 case

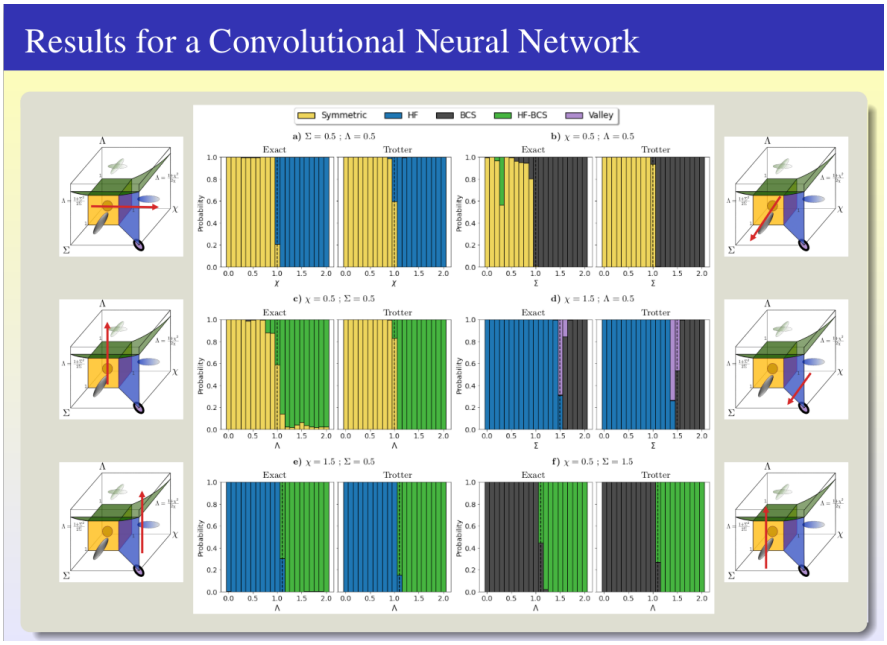
Steps to implement a Convolutional Neural Network

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.

j=2, N=8 case

Results for a Convolutional Neural Network



Álvaro Saiz, Pedro Pérez-Fernández, José-Miguel Arias, José-Enrique García-Ramos, and Lucas Lamata, "Digital quantum simulation of an extended Agassi model: Using machine learning to disentangle its phase-diagram", **Phys, Rev. C 106, 064322 (2022).**

The ELM as an approximation of the Interacting Boson Model

The ELM Hamiltonian *à la* CQF

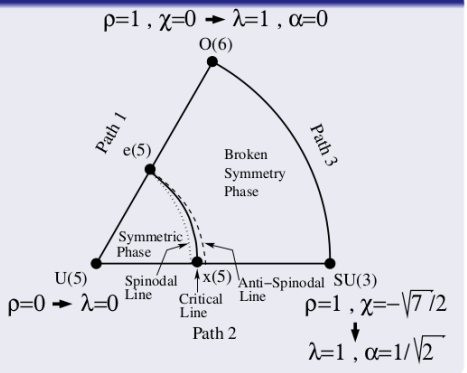
$$H = (1-\lambda)\, n_t - \frac{\lambda}{N}\, Q^{(\alpha)} \cdot Q^{(\alpha)},$$

$n_t = t^\dagger t$ and $Q^{(\alpha)} = (s^\dagger t + t^\dagger s) + \alpha(t^\dagger t)$

Equivalence with the Interacting Boson Model

$$S_+ = t^\dagger s$$
$$S_- = s^\dagger t,$$
$$S_z = \frac{1}{2}(t^\dagger t - s^\dagger s).$$

$$H_{EL} = H_L - \frac{\lambda}{N}\Big[\alpha^2(S+S_z)^2 - 2\alpha(S_x(S+S_z)+(S+S_z)S_x)\Big],$$



What a Quantum Phase Transition (QPT) is?

A QPT appears when the ground state a quantum system experiences a sudden change in its structure (order parameter) when a parameter that affects the Hamiltonian (control parameter) slightly changes around its critical value. This transitions are assumed to occurs at zero temperature.

$$\hat{H} = (1-\xi)\hat{H}_1 + \xi\hat{H}_2$$