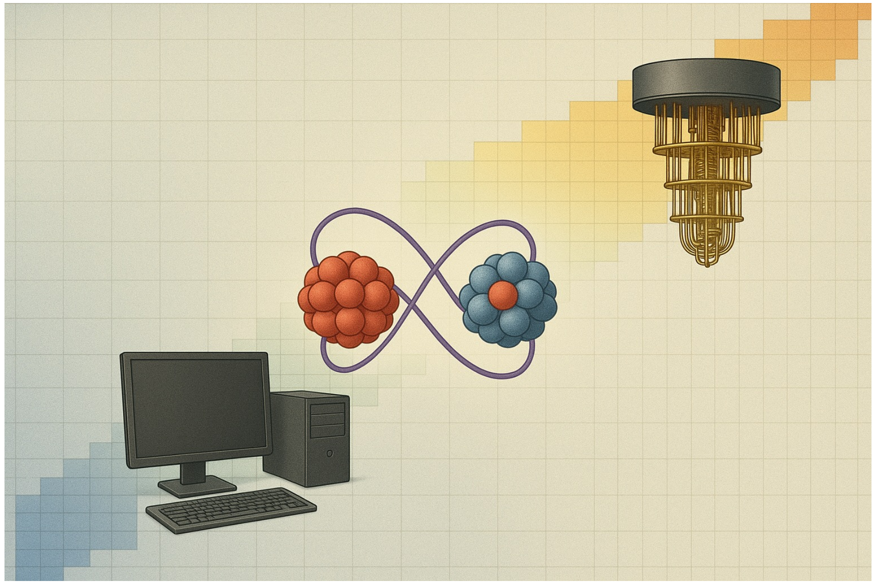
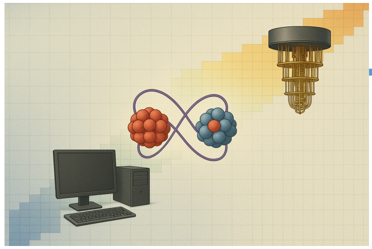
A Basic Introduction to Quantum computing: Application to nuclear physics

Denis Lacroix



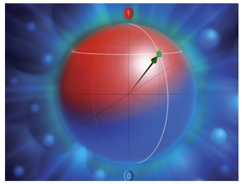
Many-body physics and QC - T. Ayral, P. Besserve, D. Lacroix, and E.A. Ruiz Guzman , Quantum computing with and for many-body physics, EPJA 59 (2023)
Symmetry and QC – D. Lacroix, A. Ruiz Guzman and P. Siwach, Symmetry breaking/symmetry preserving circuits and symmetry restoration on quantum computers, EPJA 59 (2023)
CERN Quantum Initiative – Di Meglio et al., Quantum Computing for High-Energy Physics: State of the Art and Challenges, PRX Quantum 5, 037001 (2024)



Scope of the lecture:

Part I : General aspects of quantum computing

-Some highlights on *analog* and *digital* quantum computing.
-What is a *qubit*, how to manipulate it
-Quantum gates, circuits, measurements , ...
-Noisy gates, *NISQ* versus *FTQC*



Hands-on session
First quantum circuits
with one and two qubits

Part II : Applications to nuclear physics

-The historial deuteron problem.
-Superfluid systems
-The nuclear shell-model approach on quantum computers
-Pionless Effective Field Theory on lattice
-Neutrino oscillations

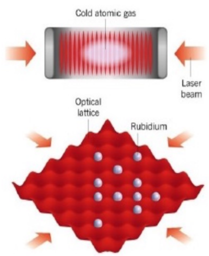
Finding the ground state
of the deuteron

What means quantum devices today

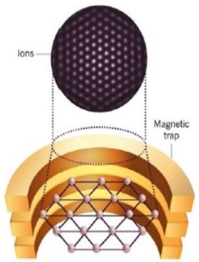
There are many types of quantum computers: ***analog versus digital quantum computers***

There are now many quantum objects one can manipulate

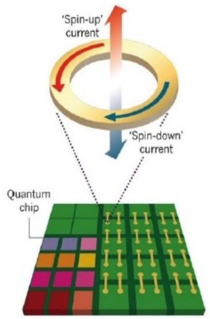
Cold atoms



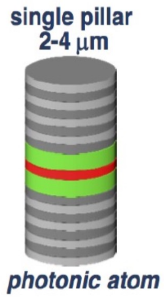
Trapped ions

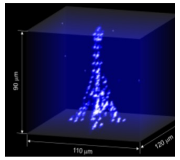


Superc. loops

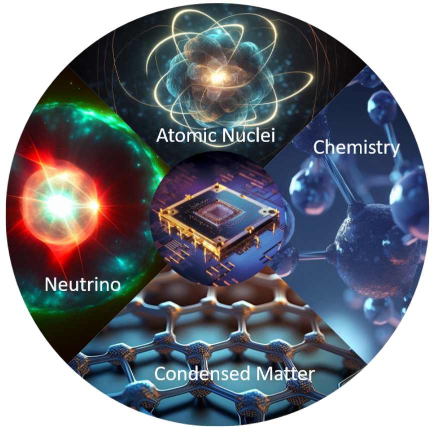


Polaritons





Atomes de Rydberg dans des pinces optiques



Analog quantum simulator

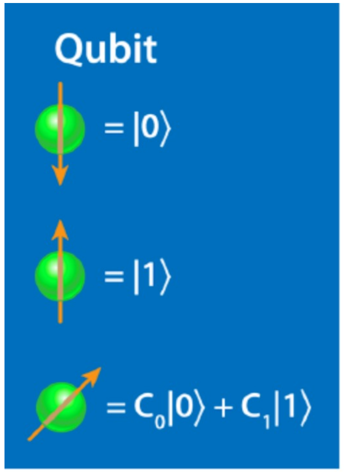
Physical problem 1 ⟷ Analog Systems ⟷ Physical problem 2

Complex problem that cannot or hardly be simulated on classical computers

Analog problem to 1 that could be tested in laboratory

⇨ Non-universal

Digital quantum simulator



⇨ Universal Quantum simulation

Quantum analogue simulation

There are many types of quantum computers: ***analog versus digital quantum computers***

A few examples

Analog quantum simulator

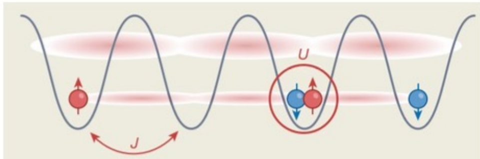
Physical problem 1 ⟷ Analog Systems ⟷ Physical problem 2

Complex problem that cannot or hardly be simulated on classical computers

Analog problem to 1 that could be tested in laboratory

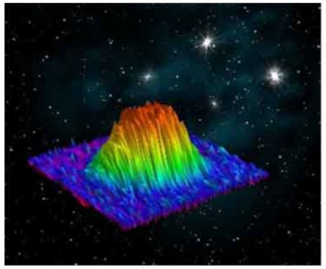
- The mapping from one physical problem to another physical problem is a delicate issue
- It strongly depends on the problem itself (non-universality)

Analog systems on lattice (Fermi-Hubbard, Schwinger model, …)



Analog simulation of astrophysics/cosmology

Ultracold Fermi gas

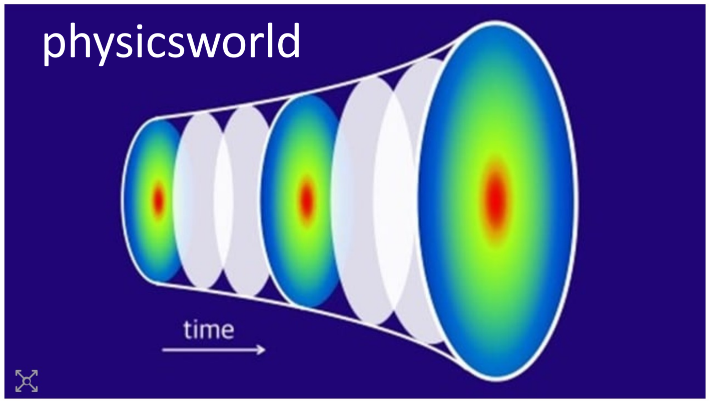


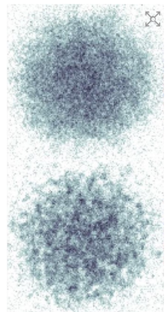
Neutron stars

Viermann et al. Nature

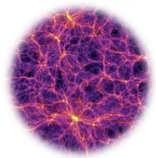
An expanding universe is simulated in a quantum droplet

22 Mar 2023 Campbell McLauchlan





Ultracold atoms



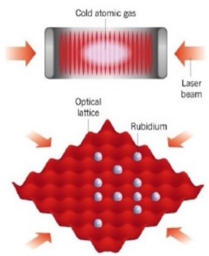
Dark matter

What means quantum devices today

There are many types of quantum computers: ***analog versus digital quantum computers***

There are now many quantum objects one can manipulate

Cold atoms



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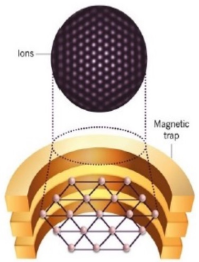

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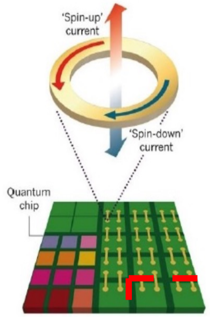

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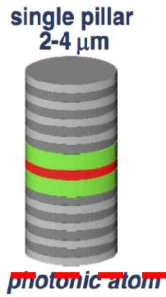

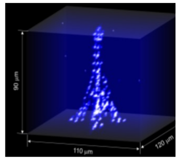

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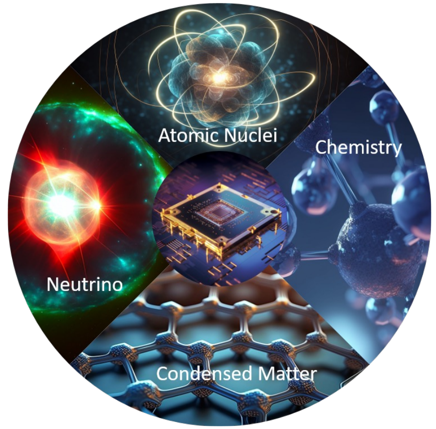

Analog quantum simulator

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Analog Systems

Physical problem 2

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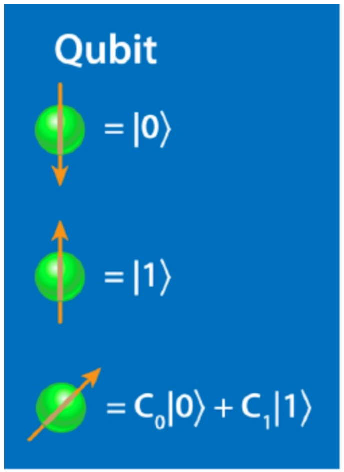
Digital quantum simulator



⇨ Universal Quantum simulation

Digital Quantum computing (basic aspects)

What can be done on a *perfect* digital quantum computer?

We can essentially solve the Schroedinger equation

Practical solution on a classical computer

$$i\hbar\frac{d}{dt}|\Psi\rangle = H|\Psi\rangle \quad \xrightarrow[\{|j\rangle\}_{j=0,\cdots}]{\text{In a basis}}$$

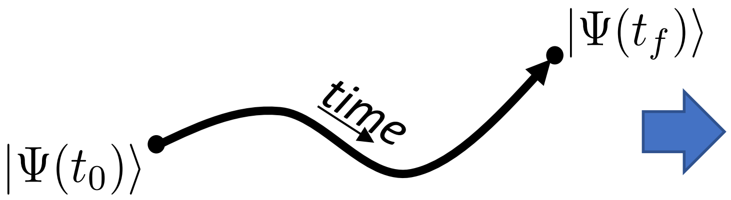
$$F_j(t) = \langle j|\Psi(t)\rangle$$

$$i\hbar\dot{F}_j(t) = \sum_i \langle j|H|i\rangle F_i(t)$$

$$i\hbar\dot{\mathbf{F}}(t) = \mathbf{H}\times\mathbf{F}(t)$$

Schroedinger Eq. is a Linear algebra problems

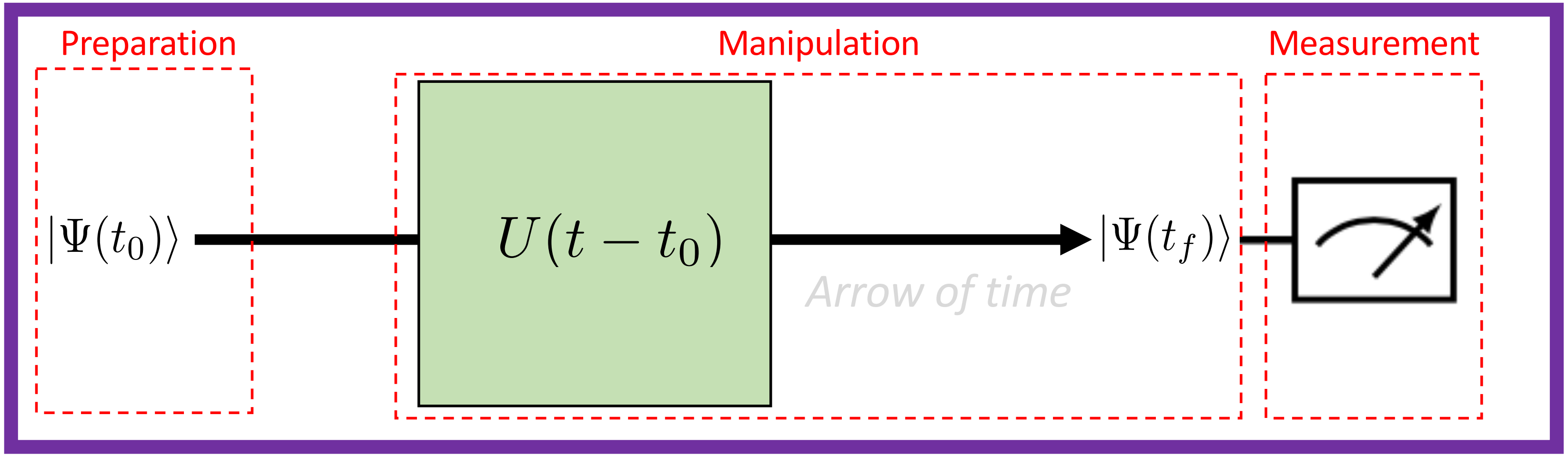
Formal solution



$$|\Psi(t)\rangle = e^{\frac{1}{i\hbar}(t-t_0)H}|\Psi(t_0)\rangle$$

$$= U(t-t_0)|\Psi(t_0)\rangle$$

Having information on the w.f. means measuring it.



Quantum Circuit

Digital Quantum Circuit

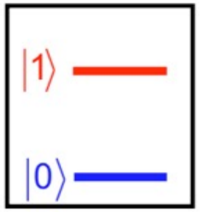
Qubit basis/quantum register

first qubit, second qubit, third qubit, ...

$$|j\rangle \Rightarrow |101000\cdots\rangle = |1\rangle \otimes |0\rangle \otimes |1\rangle \otimes \cdots$$

qubit

2 level system

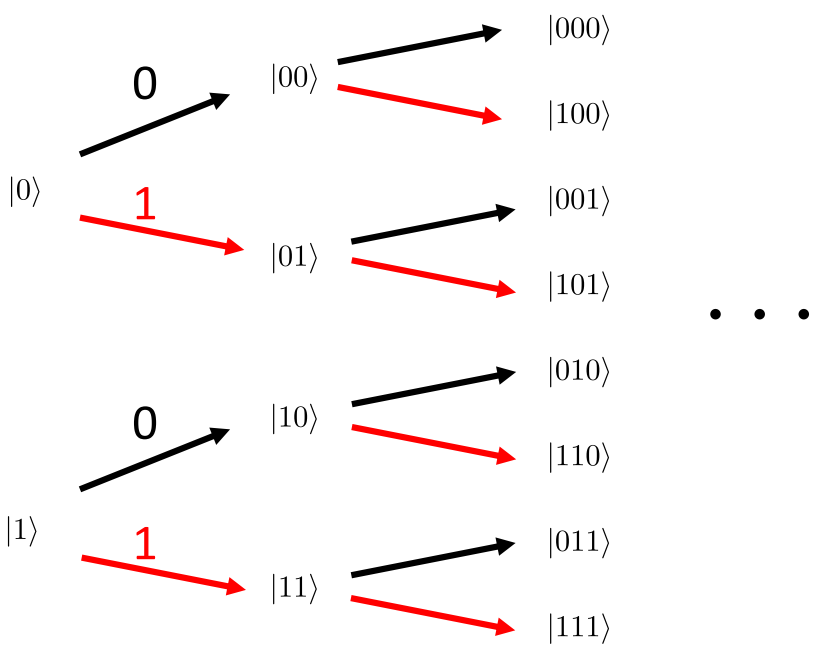


1-qubit: $|\psi\rangle = \psi_0\,|0\rangle + \psi_1\,|1\rangle$

2-qubit: $|\psi\rangle = \psi_0\,|00\rangle + \psi_1\,|01\rangle + \psi_2\,|10\rangle + \psi_3\,|11\rangle$

3-qubit: $|\psi\rangle = \psi_0|000\rangle + \psi_1|001\rangle + \psi_2|010\rangle + \psi_3|011\rangle + \psi_4|100\rangle + \psi_5|101\rangle + \psi_6|110\rangle + \psi_7|111\rangle$

1 qubit **2 qubit** **3 qubit** ...



q qubit

Computational Basis

=

qubit register

$$|s_1, \cdots, s_q\rangle$$

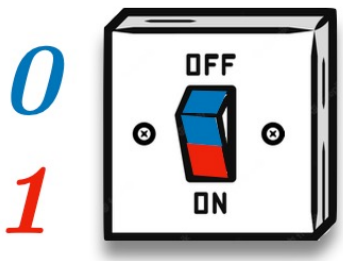
$$|0, 0, \cdots, 0, 0\rangle$$
$$|0, 0, \cdots, 0, 1\rangle$$
$$|0, 0, \cdots, 1, 1\rangle$$

...

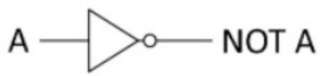
Hilbert space size scales as 2^q

Bits and classical logical gates

The Bit

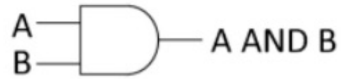


Single bit gate



A	NOT A
0	1
1	0

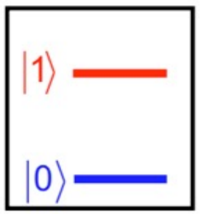
Two bits gate



A	B	A AND B
0	0	0
0	1	0
1	0	0
1	1	1

Qubits

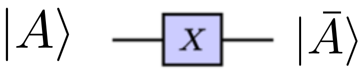
2 level system



Pauli matrices

$$\sigma_x = X = |1\rangle\langle 0| + |0\rangle\langle 1|$$
$$\sigma_y = Y = i|1\rangle\langle 0| - i|0\rangle\langle 1|$$
$$\sigma_z = Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

Single Qubit gate



Input	Output
$\|0\rangle$	$\|1\rangle$
$\|1\rangle$	$\|0\rangle$

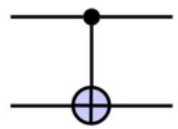
$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Two Qubits gate

Controller

Target

$|BA\rangle$



$|B'A\rangle$

Input	Output
$\|00\rangle$	$\|00\rangle$
$\|01\rangle$	$\|11\rangle$
$\|10\rangle$	$\|10\rangle$
$\|11\rangle$	$\|01\rangle$

Control

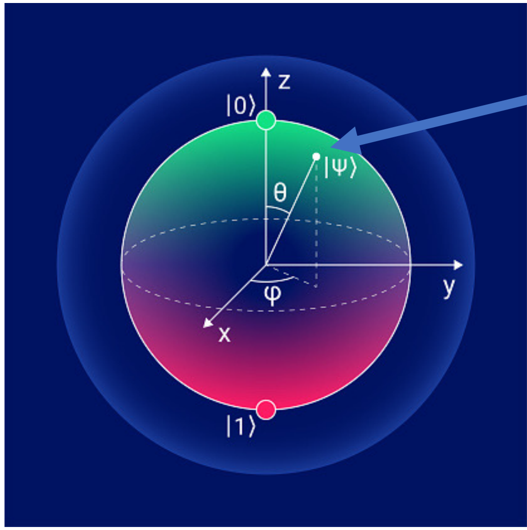
$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Because $(\psi_0, \psi_1) \in \mathbb{C}^2$ and $|\psi_0|^2 + |\psi_1|^2 = 1$, one can rewrite the qubit state as follows:

$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right) \longrightarrow |\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$

coordinates

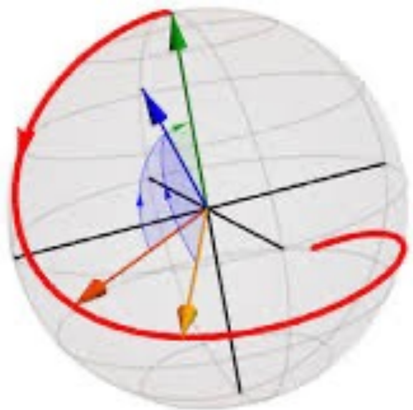
$$(\langle X\rangle, \langle Y\rangle, \langle Z\rangle)$$



Unary operations can be represented as a path in the Bloch sphere

Such state can always be obtained from 3 rotations

$$|\Psi\rangle = R_Y(\theta_1)R_Z(\theta_2)R_Y(\theta_3)|0\rangle$$



Rotations corresponds to gates

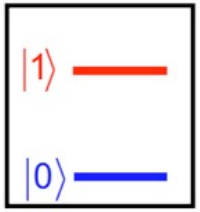
$$\boxed{R_X(\varphi) = e^{-i\varphi X/2}}$$

➡ All 1-qubit operations can be decomposed into a set of X, Y, and/or Z rotations

One qubit- some operations and measurement

qubit

2 level system



Manipulate the Qubits (Make rotations)

$|0\rangle$ Initial state

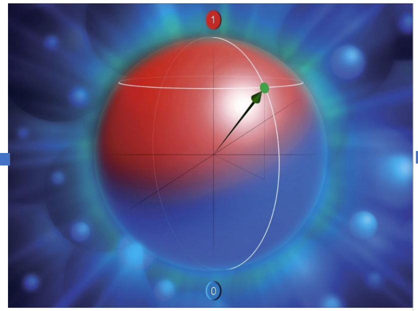


Illustration d'un qubit
CRÉDIT : MARK GARLICK / SCIENCE PHOTO LIBRA / MGA / SCIENCE PHOTO LIBRARY VIA AFP

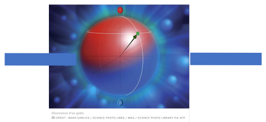
Final state $c_0|0\rangle + c_1|1\rangle$

Measure the state

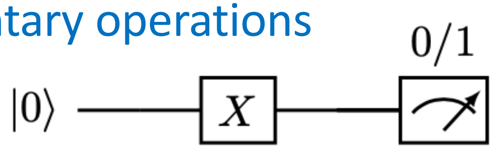
$|c_0|^2, \ |c_1|^2$

("destroy" the state)

Example of simple unary operations (gates)



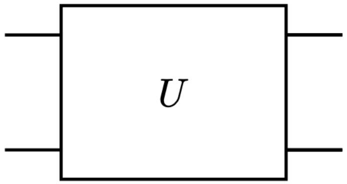
Elementary operations



Name	Symbol	Matrix	Name	Symbol	Matrix	Name	Symbol	Matrix
X	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	Y	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$	Z	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$	Phase	$P(\varphi)$	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{bmatrix}$	Universal	$U(\theta, \phi, \lambda)$	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{i\lambda}\sin\left(\frac{\theta}{2}\right) \\ e^{-i\phi}\sin\left(\frac{\theta}{2}\right) & e^{i(\phi+\lambda)}\cos\left(\frac{\theta}{2}\right) \end{bmatrix}$
X-rotation	$R_x(\theta)$	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	Y-rotation	$R_y(\theta)$	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	Z-rotation	$R_z(\theta)$	$\begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix}$

General discussion on two qubits operations

$$\alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$$



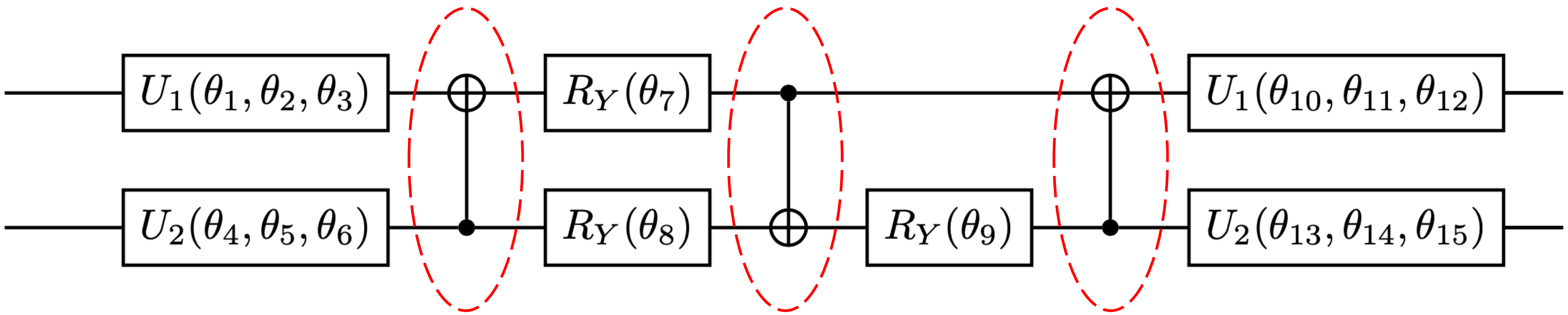
$$\alpha'|00\rangle + \beta'|01\rangle + \gamma'|10\rangle + \delta'|10\rangle$$

$$U = \begin{pmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ U_{21} & U_{22} & U_{23} & U_{24} \\ U_{31} & U_{32} & U_{33} & U_{34} \\ U_{41} & U_{42} & U_{43} & U_{44} \end{pmatrix}$$

Bin	Int
$\|00\rangle =$	$\|0\rangle$
$\|01\rangle =$	$\|1\rangle$
$\|10\rangle =$	$\|2\rangle$
$\|11\rangle =$	$\|3\rangle$

➡ In total, this gives a priori $4 + 6 \times 2 - 1 = 15$ Independent parameters

General and efficient decomposition of any *U* matrix



Binary CNOT (control-not) gate

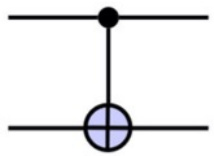
Vatan et al, Phys. Rev. A69 (2004)

(see also later: decomposition of a general circuit)

Some terminology – general aspects

Binary gates

Binary gates are operations acting simultaneously on two qubits and induced entanglement

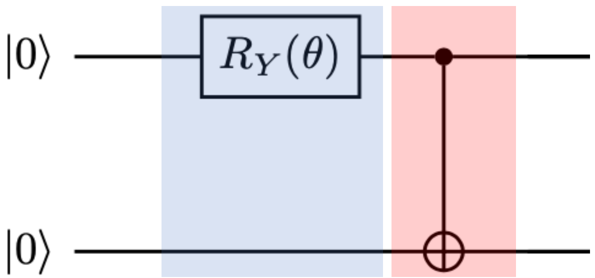


Input	Output
$\|00\rangle$	$\|00\rangle$
$\|01\rangle$	$\|11\rangle$
$\|10\rangle$	$\|10\rangle$
$\|11\rangle$	$\|01\rangle$

Control

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

Quantum circuit



Rotation

Control-X
CNOT

Step 1

$$|00\rangle \rightarrow \cos(\theta/2)|00\rangle + \sin(\theta/2)|01\rangle$$

Step 2

$$\rightarrow \cos(\theta/2)|00\rangle + \sin(\theta/2)|11\rangle$$

Indirect measurement and Born rule for measurement

If I measure 0 in first qubit → After the measurement the state collapse to $|00\rangle$

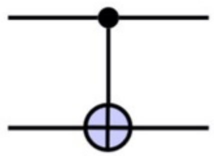
If I measure 1 in first qubit → After the measurement the state collapse to $|11\rangle$

Only one qubit needs to be measured to know the second qubit state

Some terminology – general aspects

Binary gates

Binary gates are operations acting simultaneously on two qubits and induced entanglement

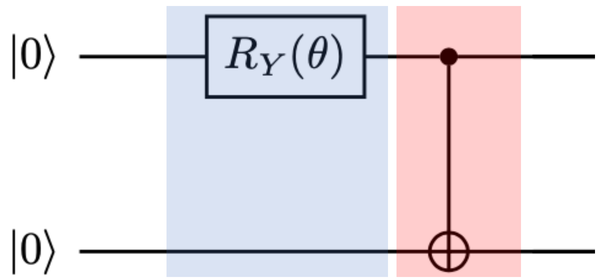


Input	Output
$\|00\rangle$	$\|00\rangle$
$\|01\rangle$	$\|11\rangle$
$\|10\rangle$	$\|10\rangle$
$\|11\rangle$	$\|01\rangle$

Control

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

Quantum circuit



Rotation

Control-X
CNOT

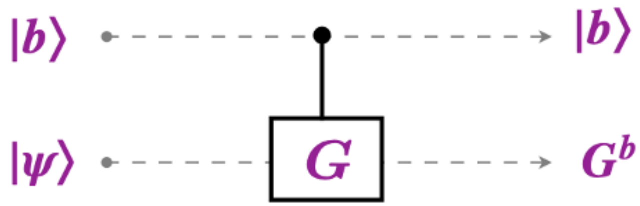
Step 1

$$|00\rangle \to \cos(\theta/2)|00\rangle + \sin(\theta/2)|01\rangle$$

Step 2

$$\to \cos(\theta/2)|00\rangle + \sin(\theta/2)|11\rangle$$

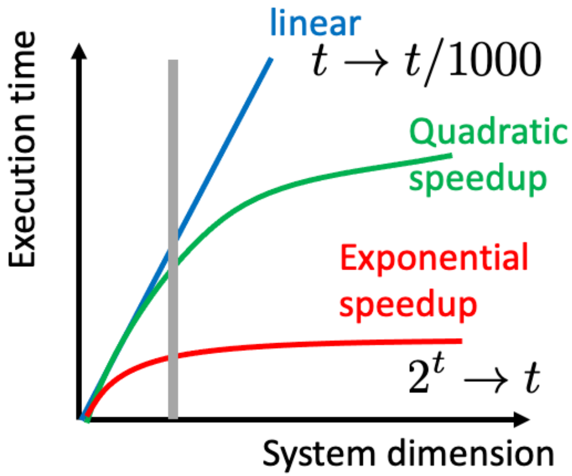
General Controlled gates (IF-THEN-ELSE)



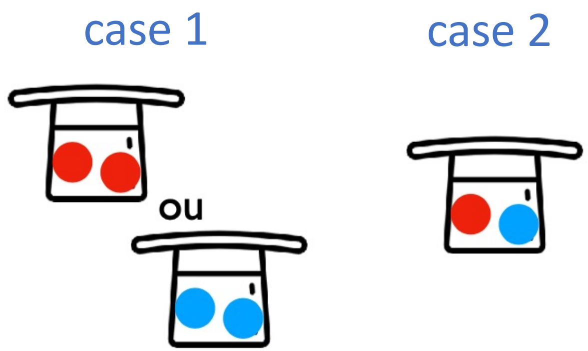
$$G^b|\psi\rangle = \begin{cases} |\psi\rangle, & \text{If } b=0 \\ G|\psi\rangle, & \text{If } b=1 \end{cases}$$

Why entangling gates are so important ?

Speedup up the solution of a problem:



A calculation that takes 1 year in a "linear" Scenario takes 24 seconds with exponential speedups!



Quantum computers promise to solve certain problem exponentially faster than classical computers

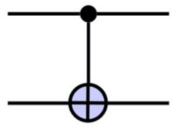
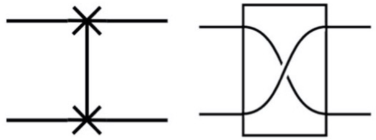
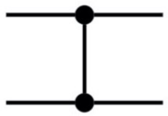
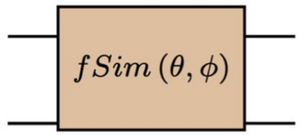
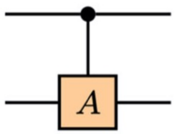
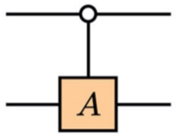
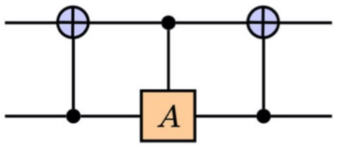
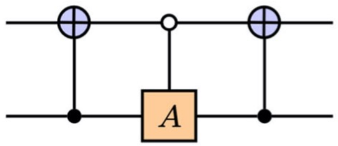
How ? $$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\bullet\;\bullet\rangle + |\bullet\;\bullet\rangle\right)$$

➡ Deutsch-Josza problem (92)

$f : \{0,1\}^n \to \{0,1\}$ Q: Is *f* constant or an equal mixing of *0* and *1 ?*

- Classically requires $1+2^{n-1}$ questions
- Quantum: requires only *1* question but *n* entangled qubits

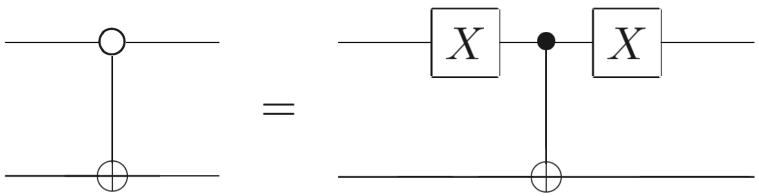
A few more example of binary gates

Name	Circuit	Matrix	Name	Circuit	Matrix
CNOT		$\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{bmatrix}$	SWAP		$\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}$
CZ		$\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{bmatrix}$	fSim		$\begin{bmatrix}1&0&0&0\\0&\cos(\theta)&-i\sin(\theta)&0\\0&-i\sin(\theta)&\cos(\theta)&0\\0&0&0&e^{i\phi}\end{bmatrix}$
a)		$\begin{bmatrix}1&0&0&0\\0&a_{00}&0&a_{01}\\0&0&1&0\\0&a_{10}&0&a_{11}\end{bmatrix}$	b)		$\begin{bmatrix}a_{00}&0&a_{01}&0\\0&1&0&0\\a_{10}&0&a_{11}&0\\0&0&0&1\end{bmatrix}$
c)		$\begin{bmatrix}1&0&0&0\\0&a_{00}&a_{01}&0\\0&a_{10}&a_{11}&0\\0&0&0&1\end{bmatrix}$	d)		$\begin{bmatrix}a_{00}&0&0&a_{01}\\0&1&0&0\\0&0&1&0\\a_{10}&0&0&a_{11}\end{bmatrix}$

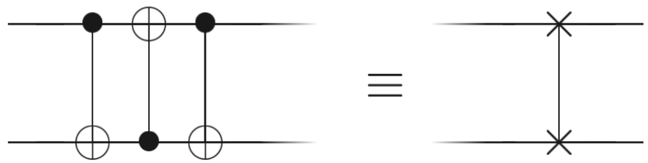
All binary circuits can be written in terms of 1 qubit operations + CNOTs

Examples

Controlled by 0



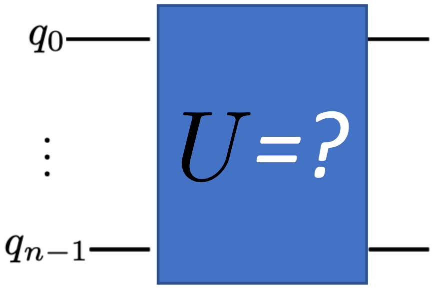
SWAP



This property turns out to remain valid for any number of qubits

More than 2 qubits: general decomposition of a unitary matrix

Decomposition of a general matrix into gates



→ All unitary matrix can be decomposed into 1-qubit operations and CNOT with arbitrary precision

Barenco et al Phys. Rev. A 52 (1995)

Some simple explanation why/how (from Nielsen & Chuang book)

All methods works iteratively and decomposes the matrix as a set of 2-level operations

Step 1 Decompose U as a product of 2 level matrices

$$U = U_\Omega \cdots U_1$$

Given rotation strategy

U_2U_1U is unitary, and thus $d'' = g'' = 0$.

$$U = \begin{bmatrix} a & d & g \\ b & e & h \\ c & f & j \end{bmatrix} \rightarrow U_1U = \begin{bmatrix} a' & d' & g' \\ 0 & e' & h' \\ c' & f' & j' \end{bmatrix} \rightarrow U_2U_1U = \begin{bmatrix} 1 & d'' & g'' \\ 0 & e'' & h'' \\ 0 & f'' & j'' \end{bmatrix} \rightarrow I \Rightarrow U = U_1^\dagger U_2^\dagger U_3^\dagger$$

$$U_1 \equiv \begin{bmatrix} \frac{a^*}{\sqrt{|a|^2+|b|^2}} & \frac{b^*}{\sqrt{|a|^2+|b|^2}} & 0 \\ \frac{b}{\sqrt{|a|^2+|b|^2}} & \frac{-a}{\sqrt{|a|^2+|b|^2}} & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad U_2 \equiv \begin{bmatrix} \frac{a'^*}{\sqrt{|a'|^2+|c'|^2}} & 0 & \frac{c'^*}{\sqrt{|a'|^2+|c'|^2}} \\ 0 & 1 & 0 \\ \frac{c'}{\sqrt{|a'|^2+|c'|^2}} & 0 & \frac{-a'}{\sqrt{|a'|^2+|c'|^2}} \end{bmatrix} \qquad U_3 \equiv \begin{bmatrix} 1 & 0 & 0 \\ 0 & e''^* & f''^* \\ 0 & h''^* & j''^* \end{bmatrix}$$

→ *U of dimension d decompose into d 2-level matrices*

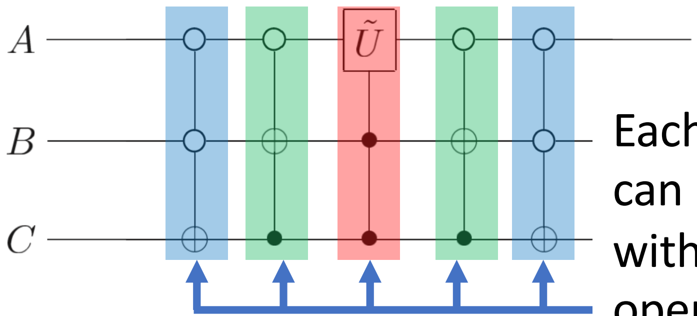
More than 2 qubits

Step 2 Decompose each 2 level matrix as a sequence of CNOT and 1 qubit gate

➡ This is done by the following scheme (Using Gray-code encoding)

$$
U = \begin{array}{c}
\begin{array}{cccccccc} |000\rangle & & & & & & & |111\rangle \end{array} \\
\left[\begin{array}{cccccccc}
a & 0 & 0 & 0 & 0 & 0 & 0 & c \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
b & 0 & 0 & 0 & 0 & 0 & 0 & d
\end{array}\right]
\begin{array}{c} |000\rangle \\ \\ \\ \\ \\ \\ \\ |111\rangle \end{array}
\end{array}
$$

A	B	C
0	0	0
0	0	1
0	1	1
1	1	1

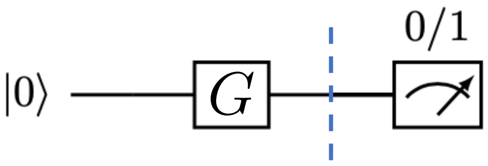


Each multiple control can be decomposed with only 1-qubit operations and CNOTs.

➡ Ultimately any n-qubit unitary matrix requires less than $(n^2 4^n)$ - 1 qubit gate and CNOTs

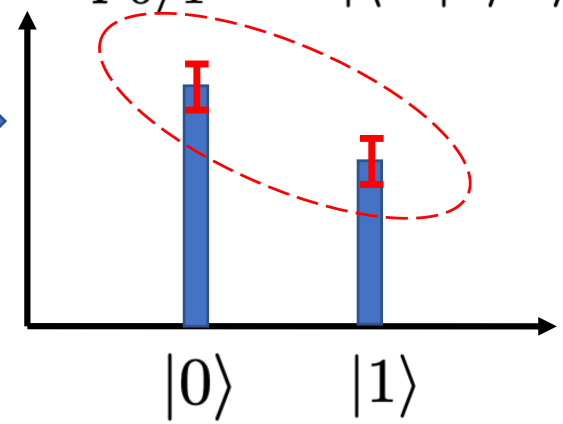
A bit more on measurement

Measurement firstly gives probabilities



$$\{b^{(n)}\} = \{0, 0, 1, \cdots ; 0\}$$

$$p_{0/1} = |\langle \Psi | 0/1 \rangle|^2$$



$$|\Psi\rangle = G|0\rangle = c_0|0\rangle + c_1|1\rangle$$

$$p_0 = \frac{1}{N_{\text{shot}}} \sum_n \delta_{0,b^{(n)}}$$

It is also one source of error (statistical one)

Two simple but important properties

➡ Measurement leads to collapse of the wave-function

Projector on channels

$$P_0 = |0\rangle\langle 0|$$

$$P_1 = |1\rangle\langle 1|$$

Measuring 0 $\quad |\Psi\rangle \Rightarrow |\Psi\rangle \longrightarrow \frac{1}{\sqrt{p_0}} P_0 |\Psi\rangle = |0\rangle$

Measuring 1 $\quad |\Psi\rangle \Rightarrow |\Psi\rangle \longrightarrow \frac{1}{\sqrt{p_1}} P_1 |\Psi\rangle = |1\rangle$

➡ Measurement can also be used to estimate observables

$$\langle Z \rangle_\Psi = \langle P_0 \rangle_\Psi - \langle P_1 \rangle_\Psi = p_0 - p_1$$

But this only works for *Z* or operators *O* such that $[O, Z] = 0$

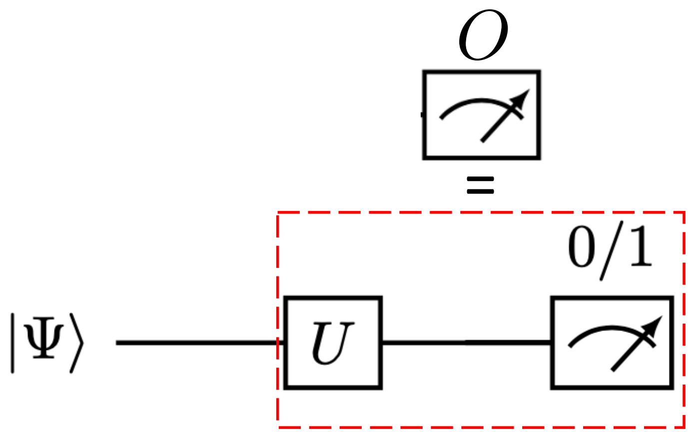
To measure an observable, one should first go in its eigenstate basis prior to the measurement:

For a general one-qubit operator *O such that*

$$O|\alpha\rangle = \lambda_\alpha|\alpha\rangle \qquad O|\beta\rangle = \lambda_\beta|\beta\rangle$$

with

$$\begin{pmatrix} |\alpha\rangle \\ |\beta\rangle \end{pmatrix} = \begin{pmatrix} & U & \end{pmatrix} \begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix}$$

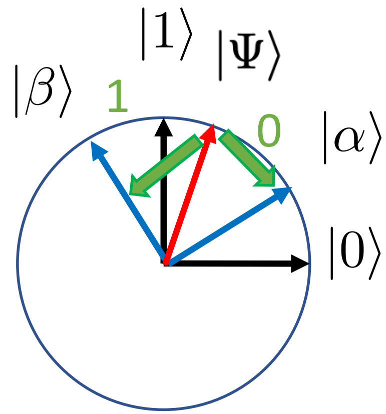


$$\{|0\rangle, |1\rangle\} \longrightarrow \{|\alpha\rangle, |\beta\rangle\}$$

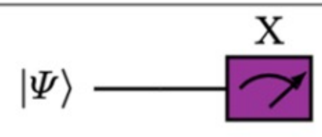
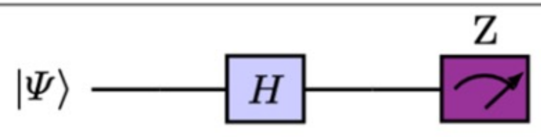
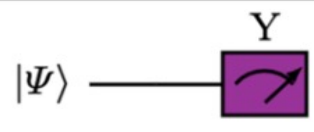
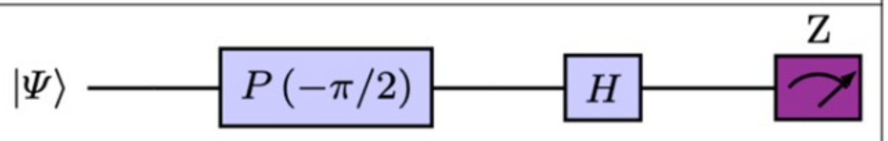
p_α p_β

$$\langle O\rangle_\Psi = \lambda_\alpha p_\alpha + \lambda_\beta p_\beta$$

It is also a tool to control the wave-function by projection/measurement



An important example: *X*, *Y*, *Z* estimates

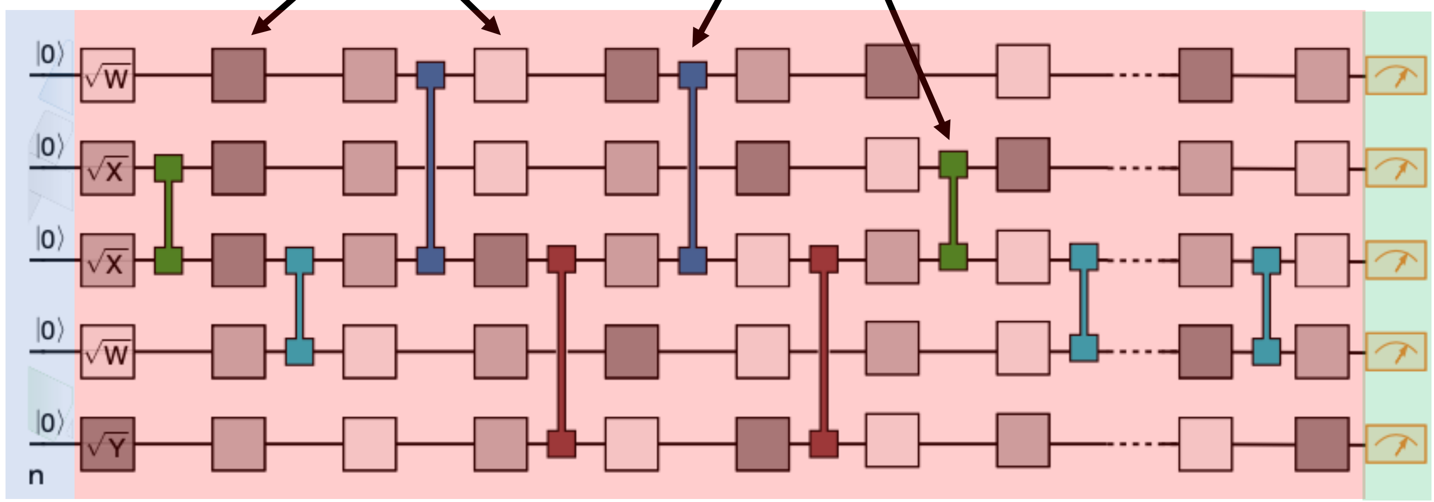
Measurement	Conversion to measurement in the Z-basis
	
	

Quantum circuits with more than one qubit

Binary gates

Unary gates

NB: all operations with more that two qubits
can be made by combination of unary and binary gates



circuit length

circuit depth

Quantum register:
Define the qubit computational basis: $|0, 0, \cdots, 0, 0\rangle$
$|0, 0, \cdots, 0, 1\rangle$
$|0, 0, \cdots, 1, 1\rangle$
$\cdots$

Hilbert space size 2^n

Quantum circuits:

Constraint: the circuit makes Unitary transformation, i.e. no loss of information

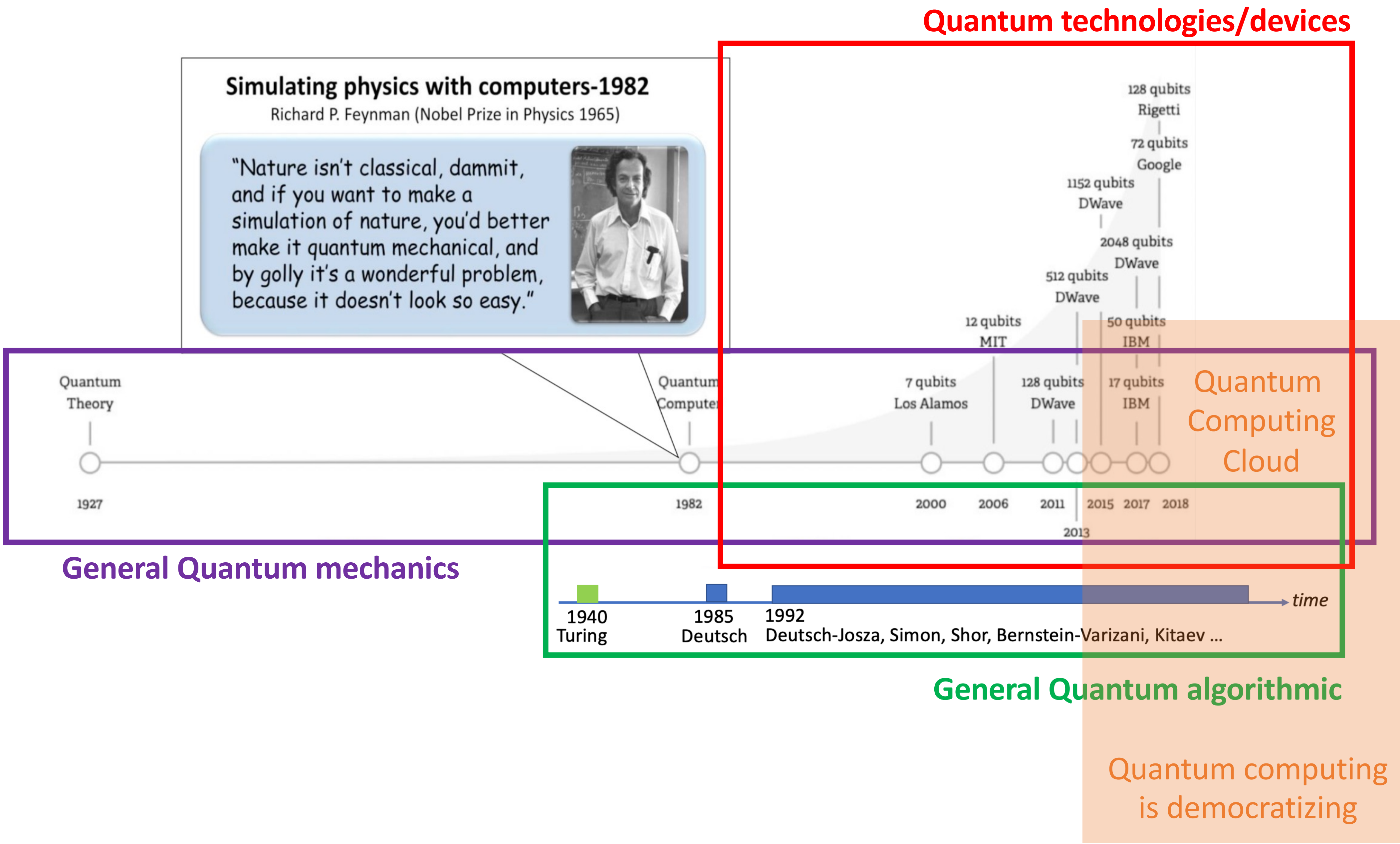
Advantage: one can imagine to do e^{itH}

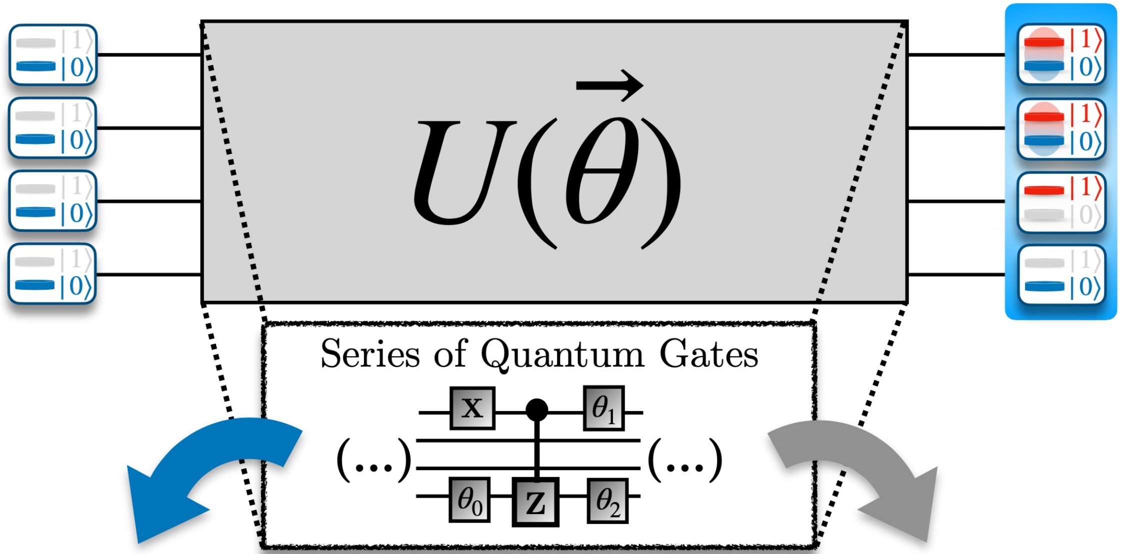
Quantum measurement of qubits – leads to a set of events In the form of bitstring

$$\sum_{i_k=0,1} a_{i_1 i_2 i_3 i_4 \dots i_{2^N}} \left| i_1, i_2, i_3 \dots i_{2^N} \right\rangle$$

Gives the $|a|^2$

Why quantum computing is becoming mature now ?





Near Term Era
Hardware limitations

Variational Quantum Eigensolver

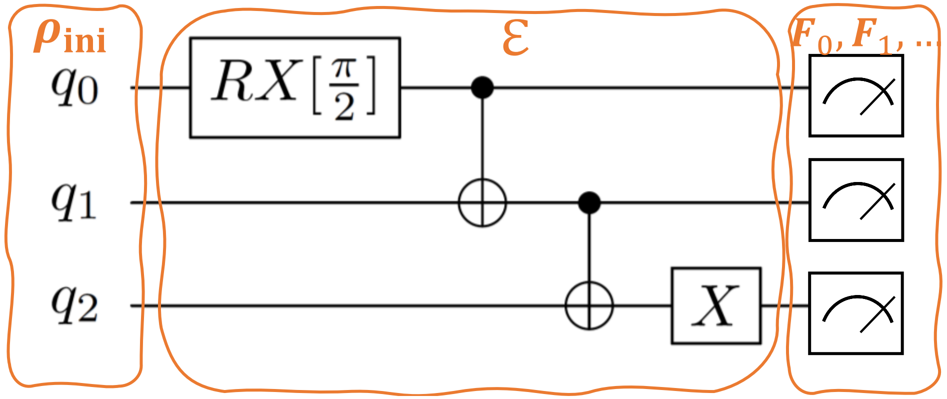
Why?

Fault Tolerant Era
No Hardware limitations

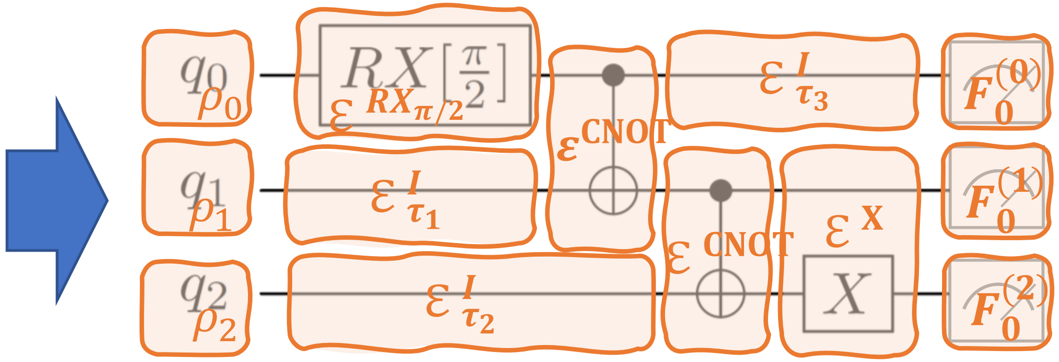
Quantum Phase Estimation

(credit: Y. Saad)

Ideal circuit



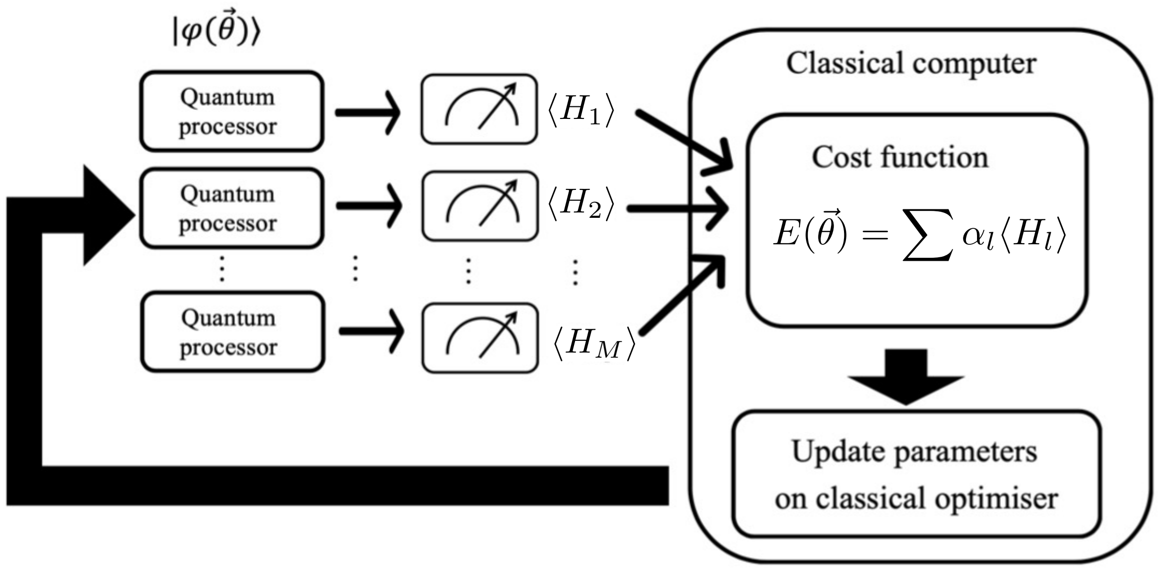
Reality circuit



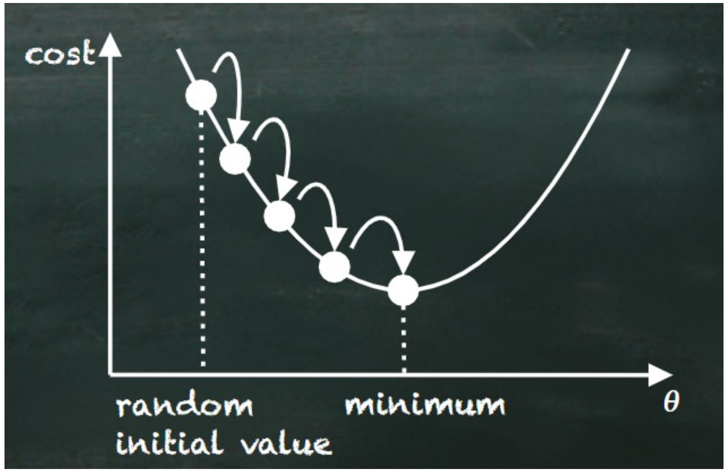
Ayral, Beserve, Lacroix, Ruiz Guzman, EPJA 2023

Main Idea of VQE

- Wave-functions can be better controlled by parametrizing them
- One can reduce the QC effort by computing expectation values of simpler operators $H = \sum \alpha_l H_l$
- The optimization task is left to a classical computer



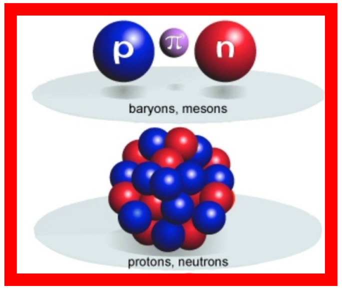
Adapted from S. Endo et al, arxiv:2011.01382
(see also K. Bharti et al., Rev. Mod. Phys. 94, 015004 (2022).

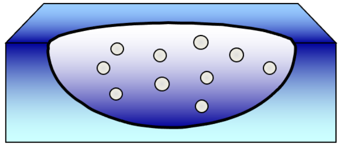


(Frank Zickert | Quantum Machine Learning)

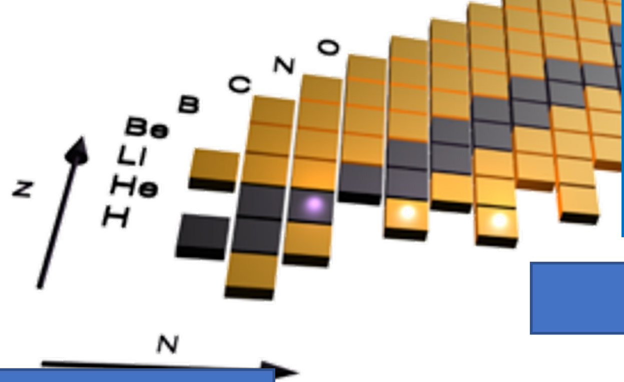
Quantum computing for the description of static and dynamical properties of atomic nuclei

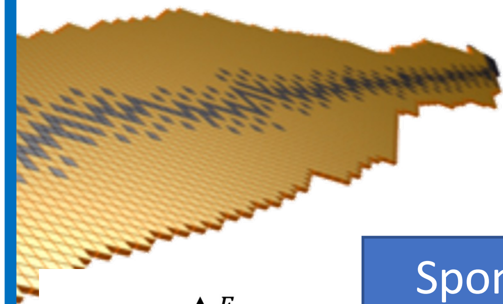
Problematic and challenges

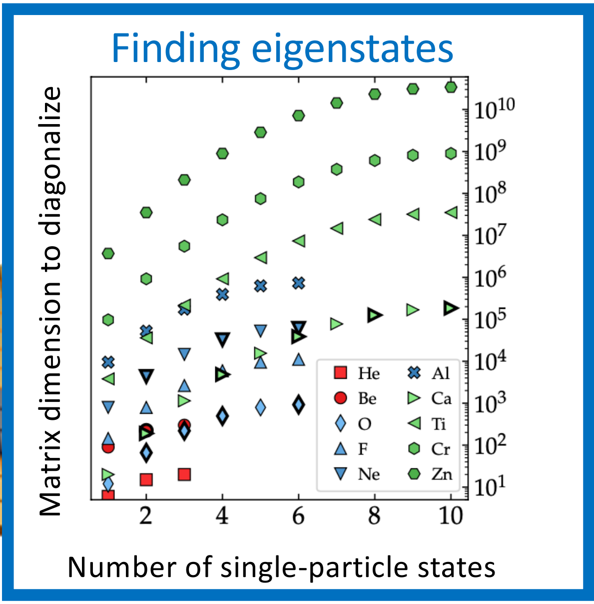


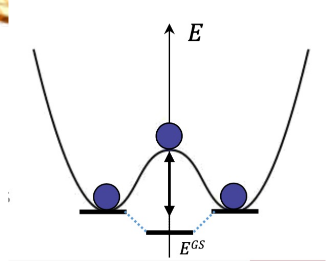


Nuclei are self-bound quantum mesoscopic systems
Nb of particles
$2 \leq A \leq 300$



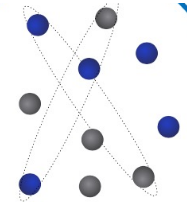






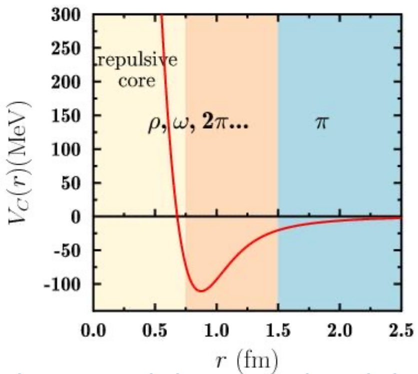
Spontaneous Broken symmetries (SB)

Small superfluid



(particle number SB)

Interaction

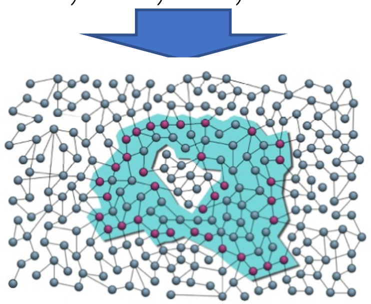


The problem is highly non-perturbative

Symmetries /Entanglement

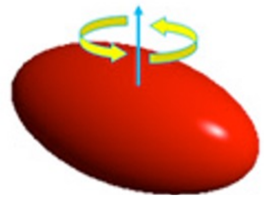
Global symmetries induce
All-to-all entanglement

$$S,\ T,\ J,\ \pi$$



Nuclei are subject to entanglement volume law
(bad candidate for Tensor Network)

Deformation can happen

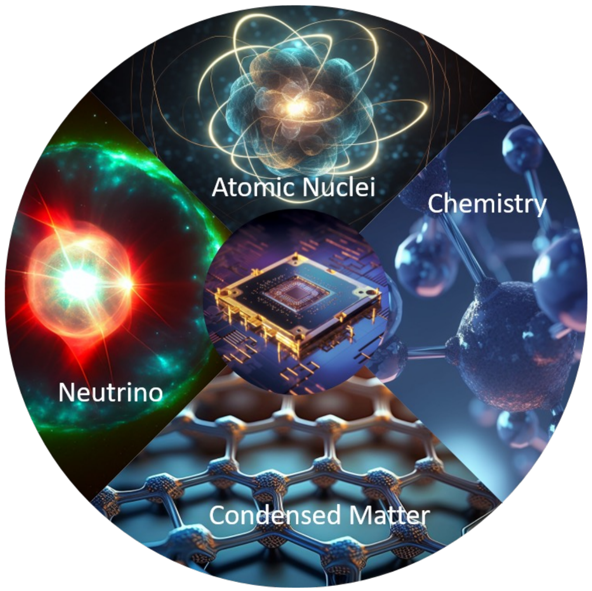


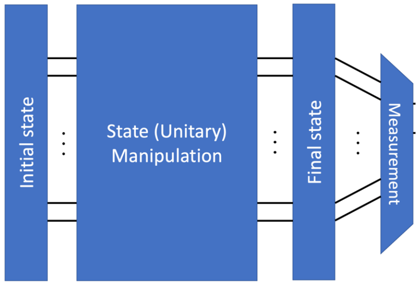
(rotational invariance SB)

...

Some Introductory Illustrations of QC applications

(Useful Quantum primitives will be introduced during the illustrations)





General strategy for quantum computing

Take a problem (classical or quantum)

↓

Encode the problem onto a set of qubits

There are many ways to encode a classical problem (phase, amplitude, time, …)

Schuld and Petruccione, Supervised learning with quantum computers (2018)

↓

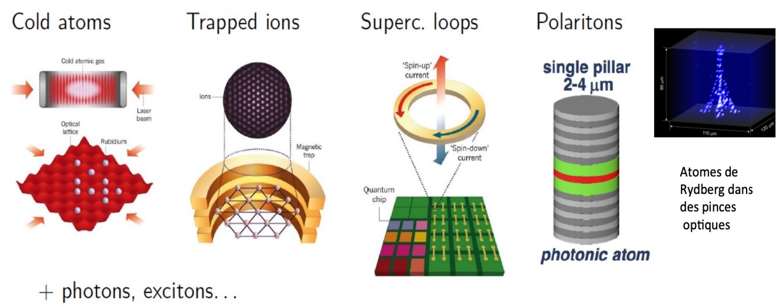
Make Quantum Computing program to solve the problem

↓ ↓

Test on a QC emulator

For instance Qiskit, pennylane, …

Test on a true QC



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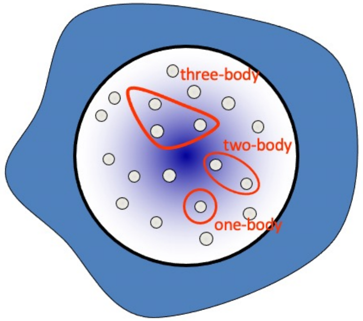

First Example:

The deuteron problem in a schematic model solved on a quantum computer

PHYSICAL REVIEW LETTERS **120,** 210501 (2018)

Editors' Suggestion Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

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[3]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[4]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
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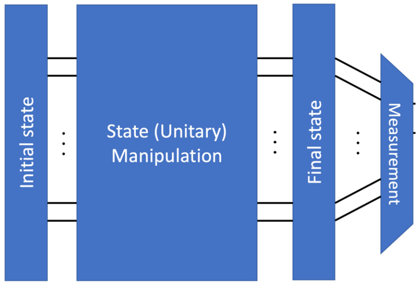
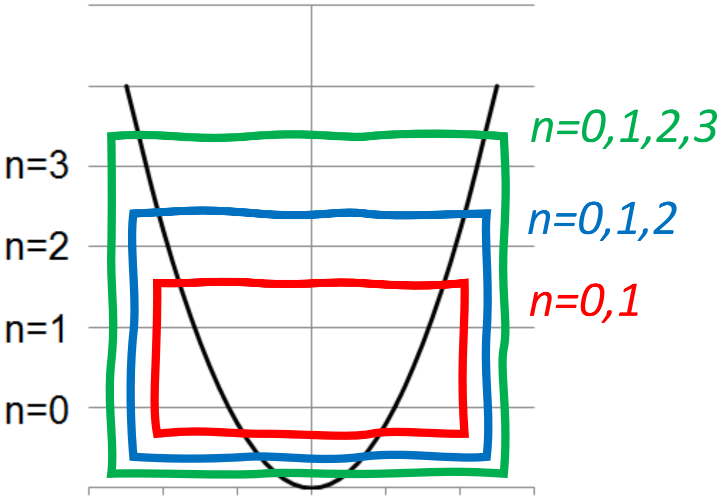


Solving the deuteron problem on a quantum computer

First step : map the deuteron problem into a simple Hamiltonian
Usable in current quantum devices



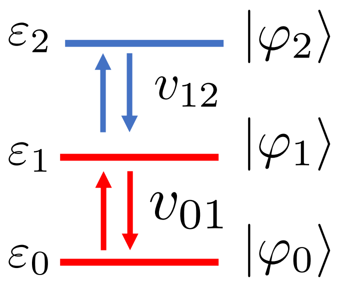
Schematic Hamiltonian in a truncated HO basis

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

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

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

The parameters are adjusted to reproduce the ground state and excited deuteron energy



On 2 levels: $H_2 = \varepsilon_0 a_0^{\dagger} a_0 + \varepsilon_1 a_1^{\dagger} a_0 + v_{01}(a_1^{\dagger} a_0 + a_0^{\dagger} a_1)$

Adding one level: $H_3 = H_2 + \varepsilon_2 a_2^{\dagger} a_2 + v_{12}(a_2^{\dagger} a_1 + a_1^{\dagger} a_2)$

. . .

Simple approach to many-problem on a quantum computer

We can assign one to each single-particle state, one qubit

$|\varphi_0\rangle \Longleftrightarrow q_0$

$|\varphi_0\rangle$ If the state is unoccupied, the qubit is in the zero state $|0\rangle$

$|\varphi_0\rangle$ If the state is occupied, the qubit is in the zero state $|1\rangle$

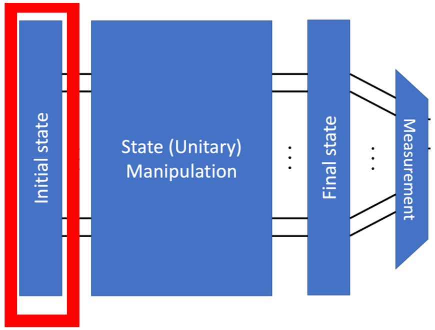
Two states = two qubits

$|\varphi_1\rangle \quad q_1$

$|\varphi_0\rangle \Longleftrightarrow q_0$

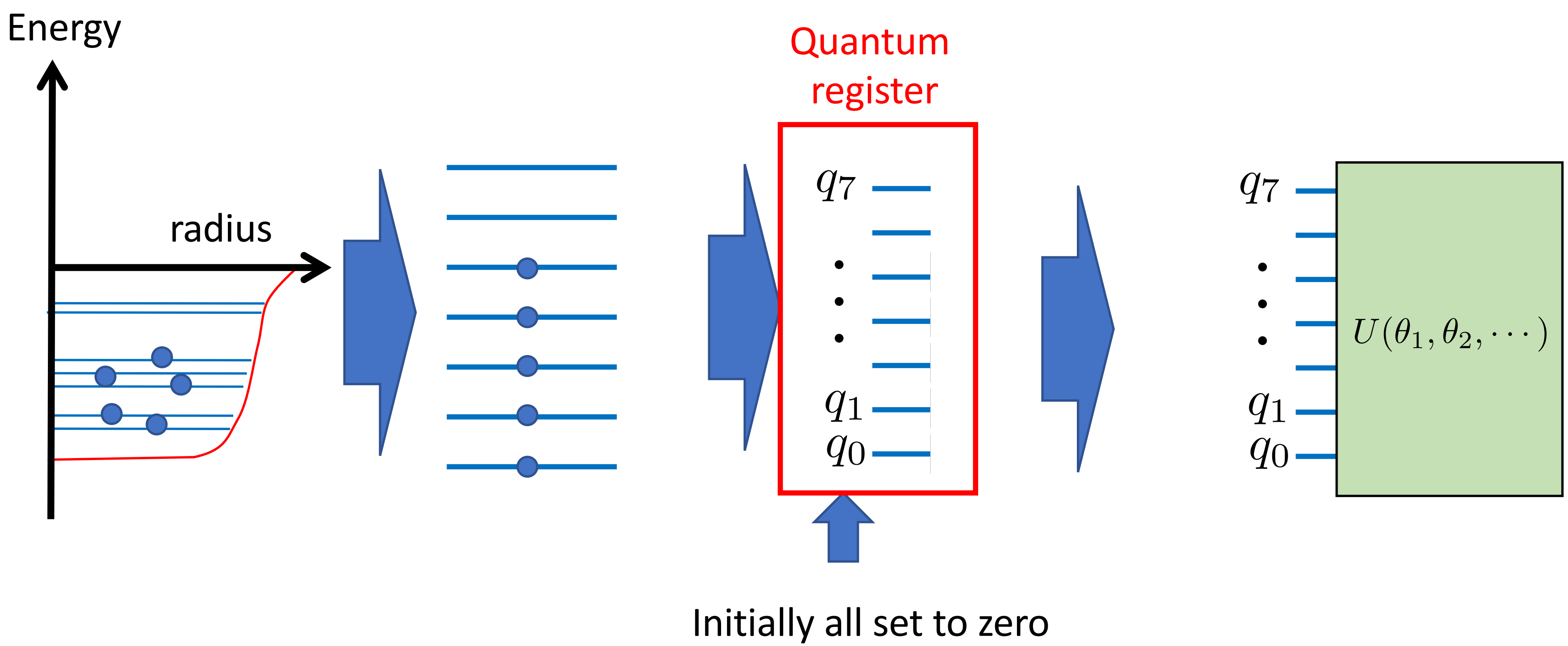
$|00\rangle$ $|01\rangle$

$|10\rangle$ $|11\rangle$



“Nuclear” Many-Body problem: initial state state preparation

Shell model on a quantum computer
in configuration interaction



One-difficulty – the antisymmetric nature of fermions

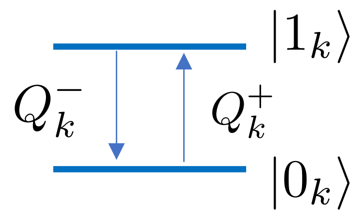
The Jordan-Wigner Transformation (JWT) solution

Mapping observable from Fock to qubit space

Mapping the Fock space into Qubits

$$|-\rangle = |0 \cdots 0\rangle$$

For qubits



For fermions

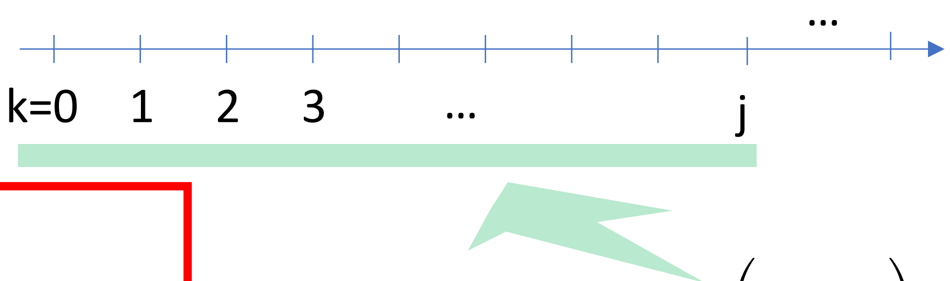
$$a_k^\dagger |-\rangle = |0 \cdots 0 \; 1_k \; 0 \cdots 0\rangle \quad \Longleftrightarrow \quad Q_k^+ = \frac{1}{2}(X_k - iY_k) = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

$$\{a_k, a_k^\dagger\} = 1 \qquad \{Q_k^-, Q_k^+\} = 1$$

Problem $\{a_k, a_l^\dagger\} = 0$ **while** $[Q_k^-, Q_l^+] = 0$

One possible solution (Jordan-Wigner transformation -1928)

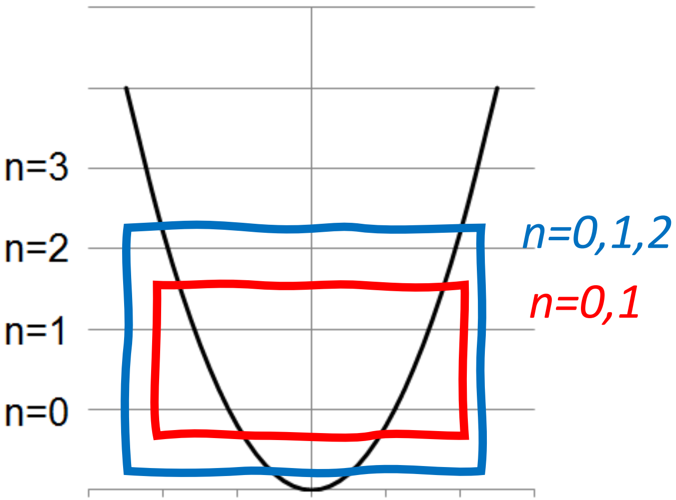
1. Order the index like in a lattice
2. Define new mapping



$$a_k^\dagger \rightarrow \left(\prod_{j<k} -Z_k \right) Q_k^+$$

The encoding is not unique:
-*Bravyi-Kitaev encoding* - Ann. Phys. 298 (2002).
-*Parity encoding* – Seeley et al, J. Chem. Phys. 137, 224109 (2012)
Encoding might lead to highly non-local multi-qubit operators!

The Jordan-Wigner method is simple and systematic, how this works:



$$\Rightarrow \quad H_2 = \varepsilon_0 a_0^\dagger a_0 + \varepsilon_1 a_1^\dagger a_0 + v_{01}(a_1^\dagger a_0 + a_0^\dagger a_1)$$

Jordan-Wigner mapping

$$a_0^\dagger \to Q_0^+$$
$$a_1^\dagger \to -Z_0 Q_1^+$$

$$(Q_k^+ Z_k = -Q_k^+)$$

$$H_2 = \frac{\varepsilon_0}{2}(I - Z_0) + \frac{\varepsilon_1}{2}(I - Z_1) + v_{01}(X_0X_1 + Y_0Y_1)$$

$$\boxed{H_2 = 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304(X_0X_1 + Y_0Y_1)}$$

Adding a qubit: $a_2^\dagger \to Z_0 Z_1 Q_2^+$

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119(X_1X_2 + Y_1Y_2)$$

$$\cdots$$

A few simple but important remarks

$$\boxed{H_2 = 5.906709 I + 0.218291 Z_0 - 6.125 Z_1 - 2.143304(X_0 X_1 + Y_0 Y_1)}$$

$$H = \sum_{i \in \mathcal{G}} c_i P_{i_0} \cdots P_{i_{n_q}} \qquad P \in \{I, X, Y, Z\}$$

hermitian
But not unitary

Pauli String
Unitary operator

The group *G* has ~*4^n* elements

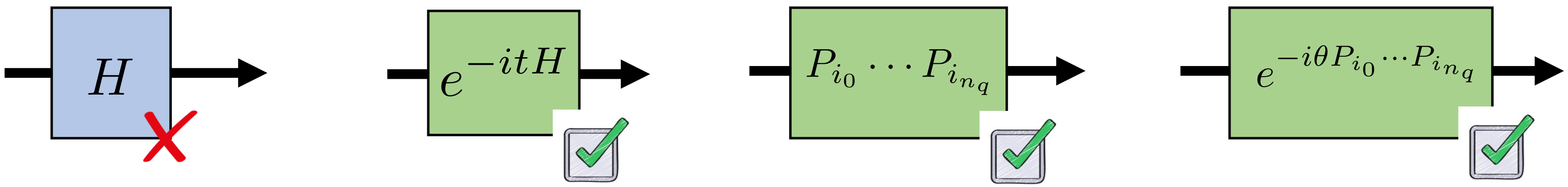
➡ Pauli-string decomposition is universal

This is the essence of quantum tomography

For one qubit $\rho = \frac{1}{2}\left[\mathrm{Tr}(\rho) I + \mathrm{Tr}(\rho X) X + \mathrm{Tr}(\rho Y) Y + \mathrm{Tr}(\rho Z) Z\right]$

But tomography has an exponential cost with the number of qubits.

➡ Given *H*, which operation can be a priori implemented on a quantum computer?



Practical solution on a quantum computer

What problem exactly are we trying to solve?

$$H_2 = a_0 I + a_1 Z_0 + a_2 Z_1 + a_3 (X_0 X_1 + Y_0 Y_1)$$

$$\Rightarrow H = \begin{array}{cc} \begin{pmatrix} a_0 + a_1 + a_2 & 0 & 0 & 0 \\ 0 & a_0 + a_1 - a_2 & 2a_3 & 0 \\ 0 & 2a_3 & a_0 - a_1 + a_2 & 0 \\ 0 & 0 & 0 & a_0 - a_1 - a_2 \end{pmatrix} & \begin{array}{c} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \end{array}$$

On a classical computer

We diagonalize $\Rightarrow |GS\rangle = \alpha|10\rangle + \beta|10\rangle$

In Fock space

In qubit space

$$|\Psi(\theta)\rangle = e^{i\theta(a_1^\dagger a_0 - a_0^\dagger a_1)} a_0^\dagger |00\rangle \Rightarrow |\Psi(\theta)\rangle = e^{i(\theta/2)(X_0 Y_1 - Y_0 X_1)} X_0 |00\rangle$$

The ground state can be found by minimizing the energy: $E(\theta) = \langle \Psi(\theta) | H_2 | \Psi(\theta) \rangle$

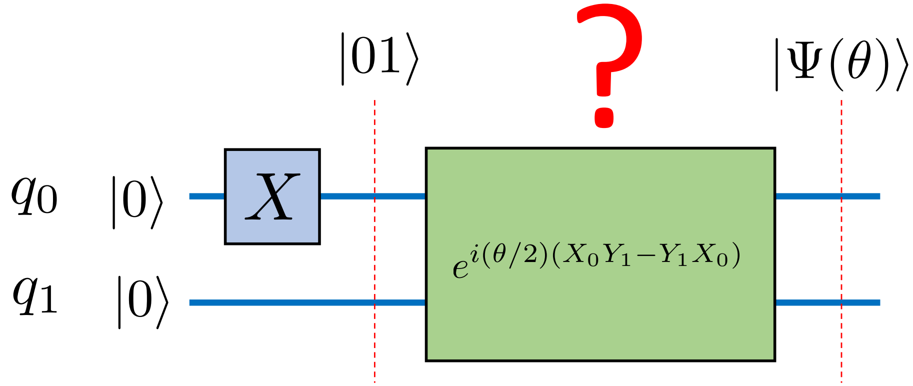
A few simple but important remarks

What problem exactly are we trying to solve?

$$H_2 = a_0 I + a_1 Z_0 + a_2 Z_1 + a_3 (X_0 X_1 + Y_0 Y_1)$$

State preparation

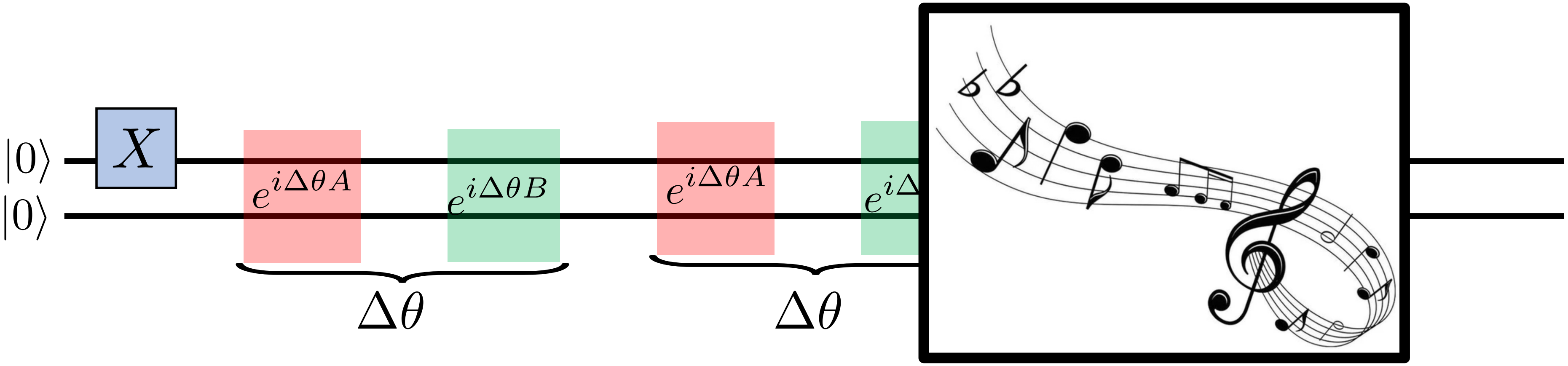
$$|\Psi(\theta)\rangle = e^{i(\theta/2)(X_0 Y_1 - Y_0 X_1)} X_0 |00\rangle$$



Standard strategy

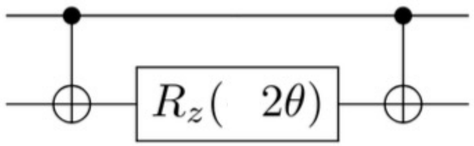
The (first order) Trotter-Suzuki formula

$$\left\| e^{it(A+B)} - \left[e^{i\delta t A/n} e^{i\delta t B/n} \right]^n \right\| \leq \frac{\delta t^2}{2n} \| [A, B] \| \leq \epsilon$$



General method to obtain a circuit

$$e^{i\theta Z_0 Z_1}$$



Other circuits can be obtained using

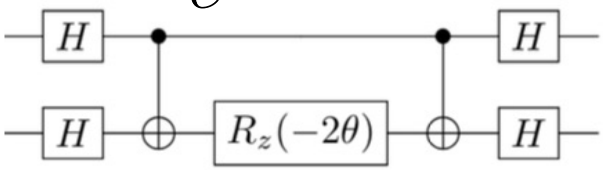
$$HXH = Z$$

$$(HS^\dagger)Y(SH) = Z$$

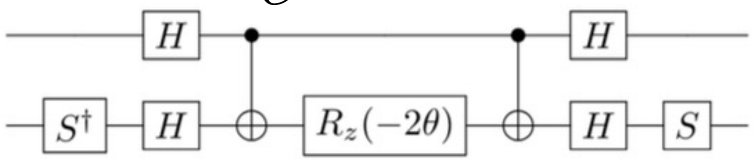
Z-basis $\xrightarrow{H}$ X-basis $\xrightarrow{H}$ Z-basis

Z-basis $\xrightarrow{S^\dagger H}$ X-basis $\xrightarrow{HS}$ Z-basis

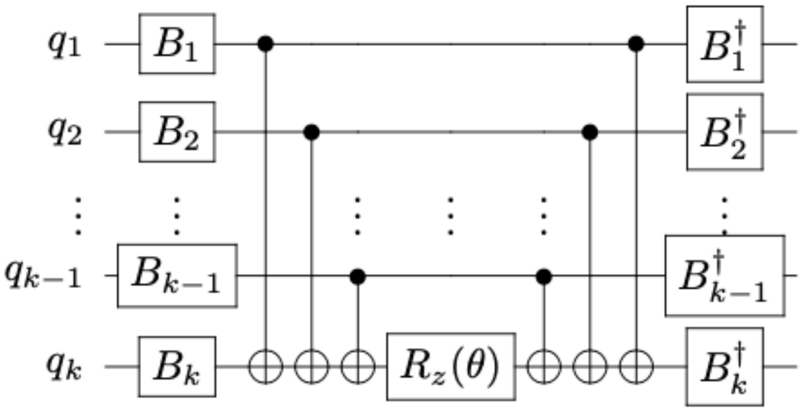
$$e^{i\theta X_0 X_1}$$



$$e^{i\theta X_0 Y_1}$$



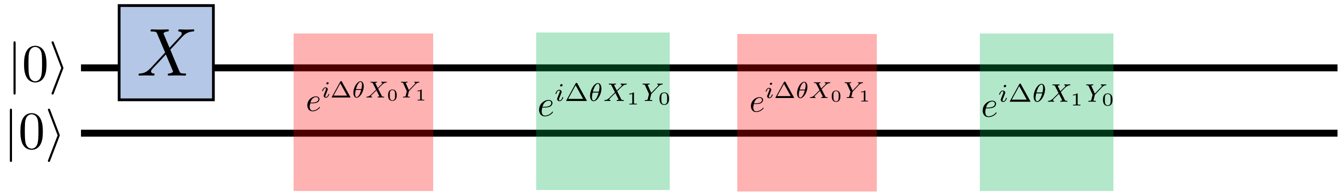
General staircase circuit



P_i	B_i	Check: $B_i P_i B_i^\dagger$
Z	I	Z
X	H	Z
Y	$HS^\dagger$	Z

(courtesy to R. Bocquet)

Circuit length

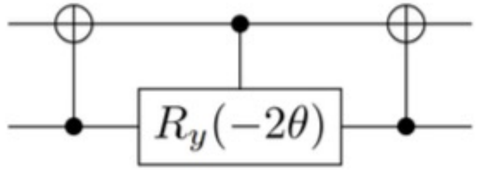


1 qubit gate	+1	+7	+7	+7	+7	. . .
CNOT gates		+2	+2	+2	+2	

Circuits are not unique !

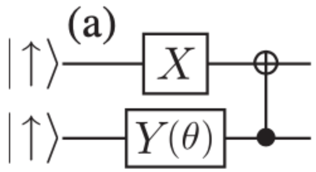
Can be made with three control gates
and one rotation only

$$e^{-i\theta(Y_1X_2-X_1Y_2)}$$



The circuit has been further reduced to

Dumitrescu et al, PRL 120 (2018)



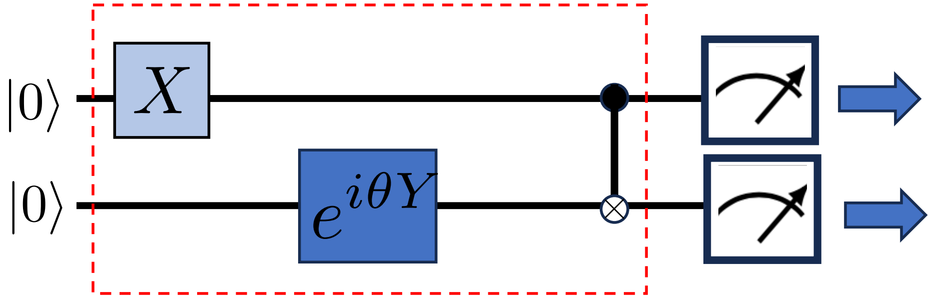
2 gates
1 CNOT

A few simple but important remarks

$$H_2 = a_0 I + a_1 Z_0 + a_2 Z_1 + a_3 (X_0 X_1 + Y_0 Y_1)$$

Energy evaluation

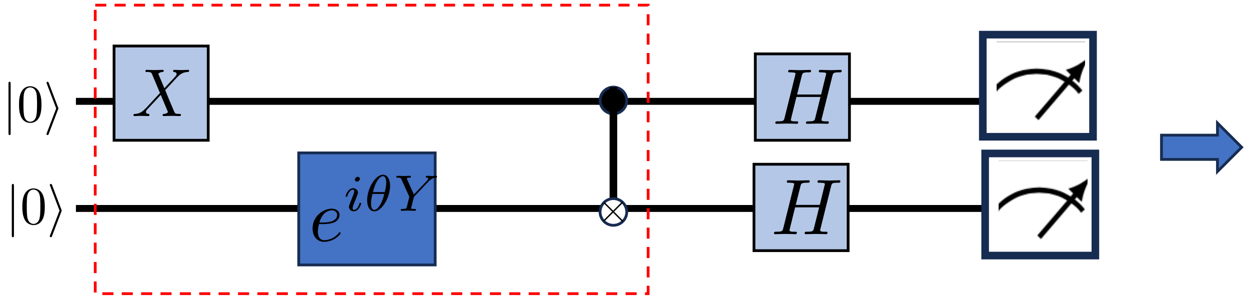
Circuit 1



$$\langle Z_0 \rangle_\theta = p_0 - p_1$$

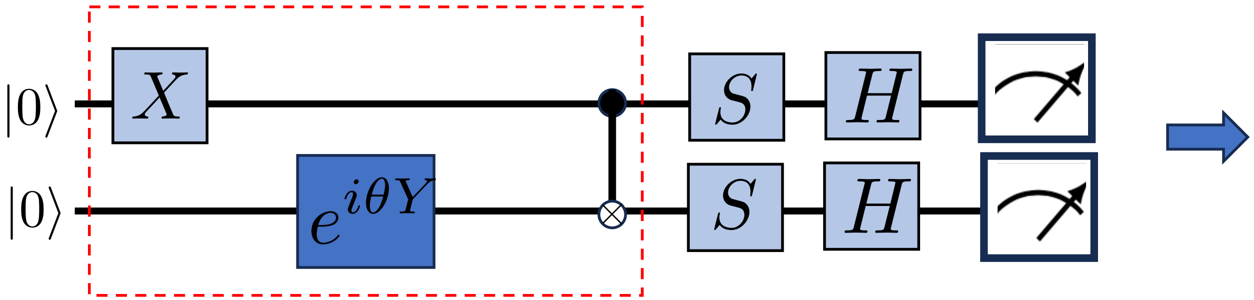
$$\langle Z_1 \rangle_\theta = p_0 - p_1$$

Circuit 2



$$\langle X_0 X_1 \rangle$$

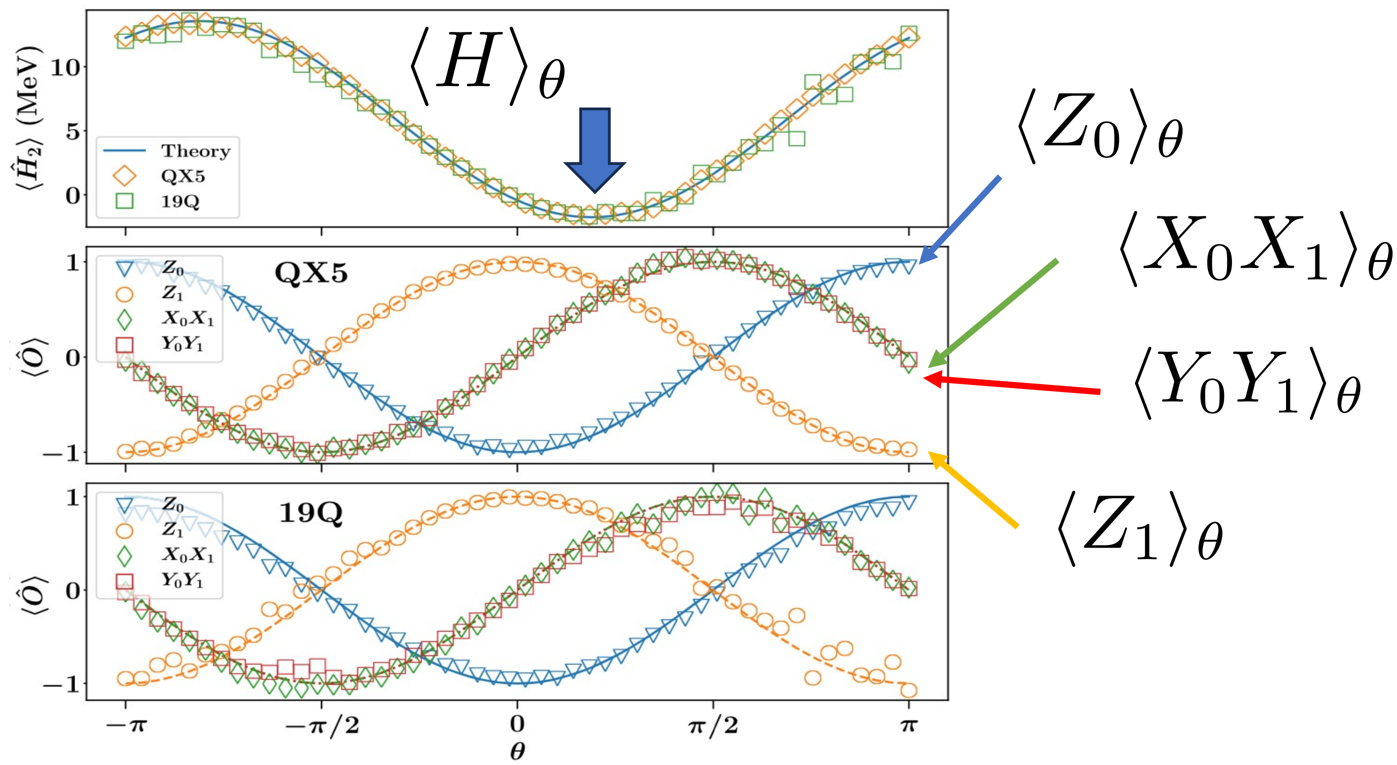
Circuit 3



$$\langle Y_0 Y_1 \rangle$$

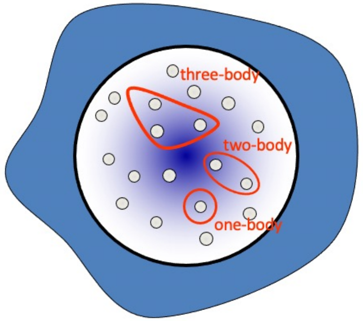
Energy can be reconstructed

$$E_\theta = a_0 + a_1\langle Z_0\rangle_\theta + a_2\langle Z_1\rangle_\theta + a_3(\langle X_0X_1\rangle_\theta + \langle Y_0Y_1\rangle_\theta)$$

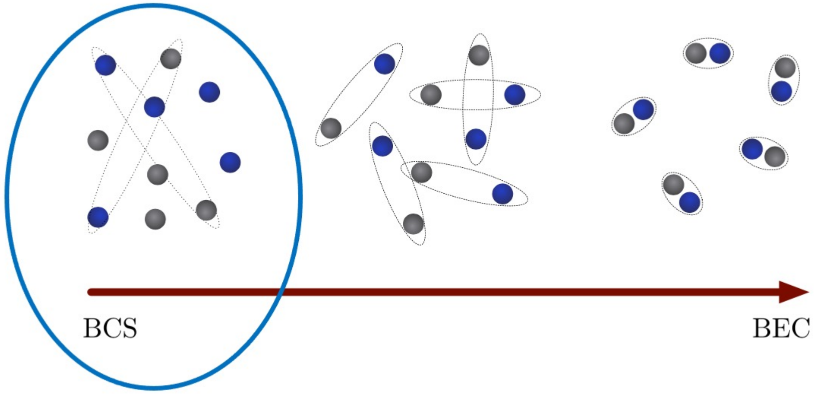


Dumitrescu et al, Phys. Rev. Lett. 120 (2018)

See tutorial!



Second Example:
Treating superfluid systems



This problem is an archetype of spontaneous symmetry breaking/symmetry restoration in nuclear physics.

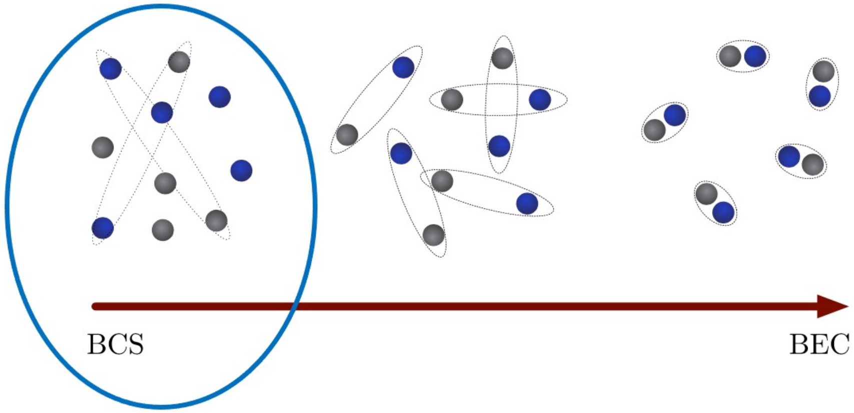
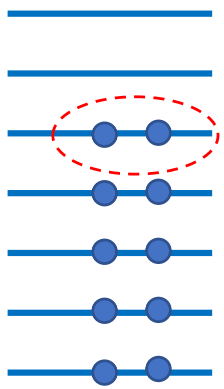
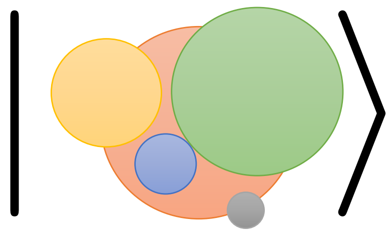


Illustration with the pairing Hamiltonian

Illustration with the Richardson Hamiltonian



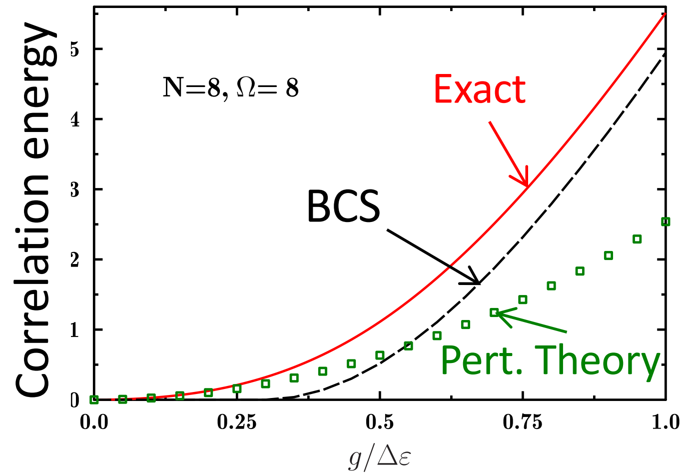
$$H_{\mathrm{P}} = \sum_{i>0} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) - g \sum_{i,j>0} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j$$



Example $|\Phi_0\rangle = \Pi_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$

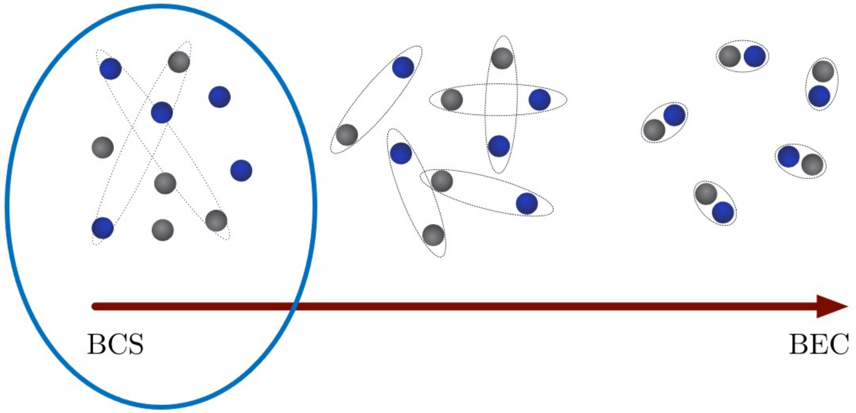
⇒ Mixes states with 0, 2, 4, … particles

The particle number - U(1) symmetry) is broken



How to encode the Hamiltonian and prepare this state on a quantum computer ?

Illustration with the pairing Hamiltonian



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

Again qubit ordering,
is crucial!

First step Fermion to qubit mapping

States labels $\quad i \quad \bar{i} \quad \dots$

Qubits labels $\quad 0 \quad 1 \quad 2 \quad \dots \quad n \quad n+1$

Jordan-Wigner trans:

$$a_i^\dagger a_i \Rightarrow \frac{1}{2}(I_n - Z_n)$$

$$a_i^\dagger a_{\bar{i}}^\dagger \Rightarrow Q_n^+ Q_{n+1}^+$$

with $\quad Q_n^+ = \frac{1}{2}(X_n - iY_n)$

Second step: prepare the wave-function with a circuit

$$|\Phi_0\rangle = \Pi_i (u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle$$

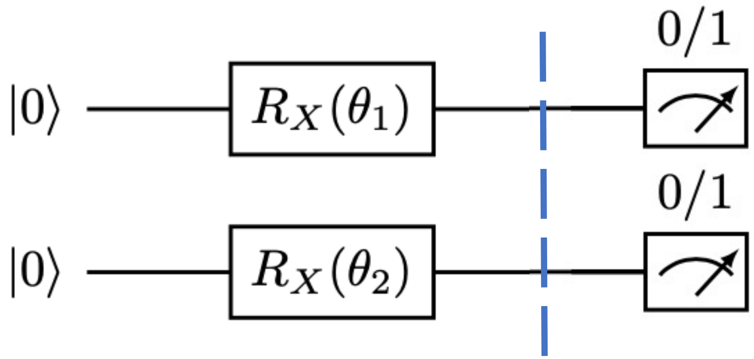
Consider one pair

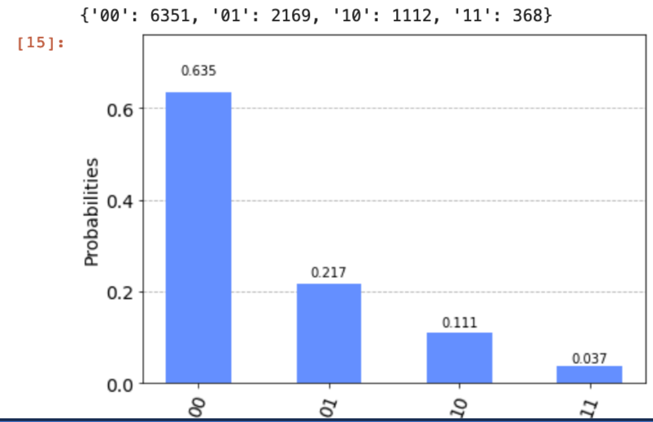
$$\Rightarrow (u_n + v_n Q_n^+ Q_{n+1}^+)|00\rangle = u_n|00\rangle + v_n|11\rangle$$

Equivalent to a generalized Bell state)

Preparing a Bell (Pairing state)

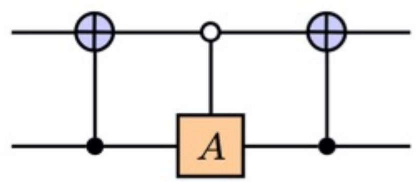
Independent particle





$$(\alpha_1|0\rangle + \beta_1|1\rangle) \otimes (\alpha_2|0\rangle +$$

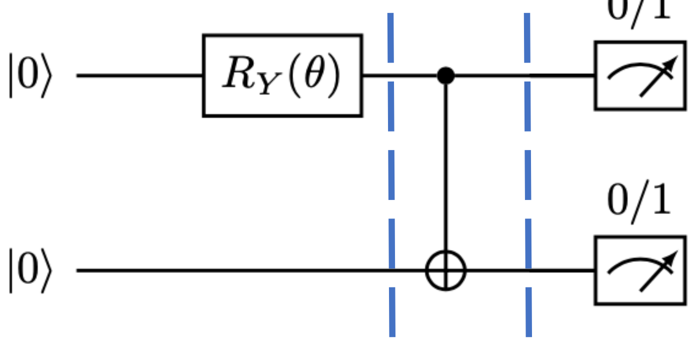
Again the circuit is not unique



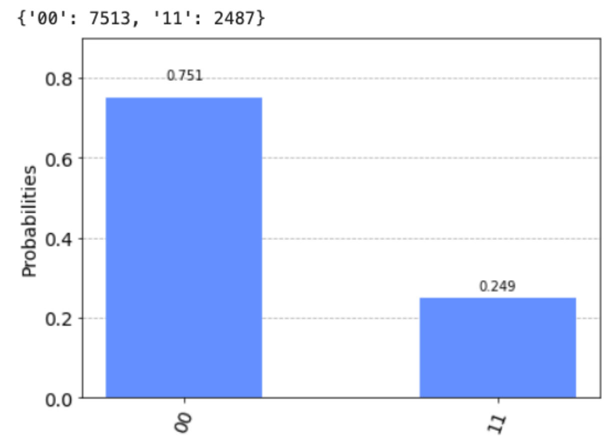
$$\begin{bmatrix} a_{00} & 0 & 0 & a_{01} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ a_{10} & 0 & 0 & a_{11} \end{bmatrix}$$

Entangled/correlated state

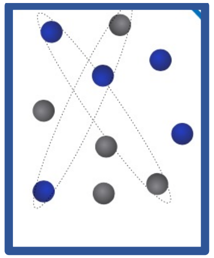
$$(\alpha|0\rangle + \beta|1\rangle) \otimes |0\rangle$$



$$(\alpha|00\rangle + \beta|11\rangle)$$

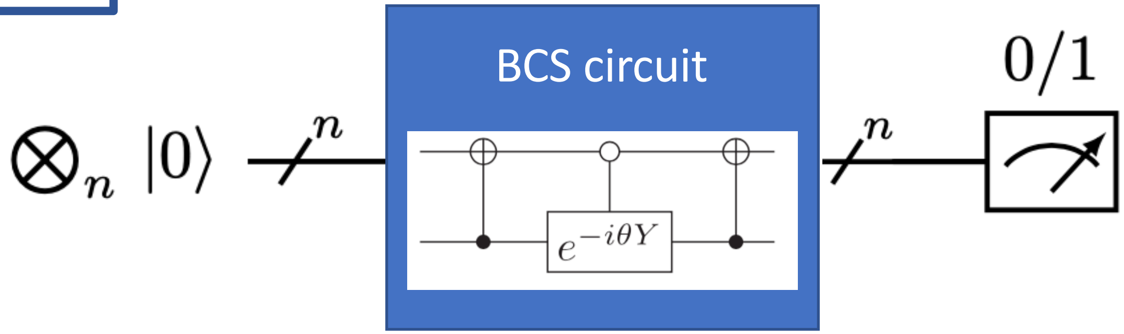


Here I created a Bell state

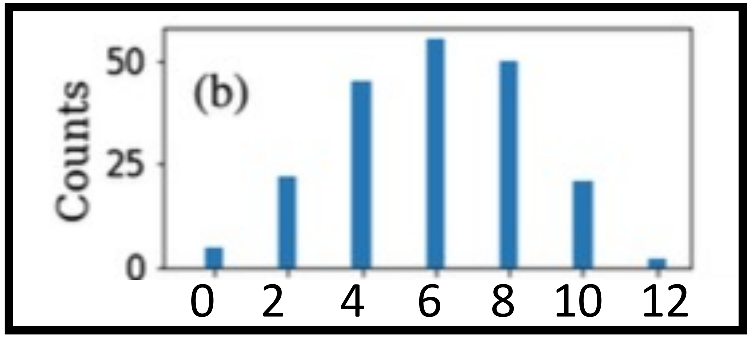


Quantum computing for atomic nuclei

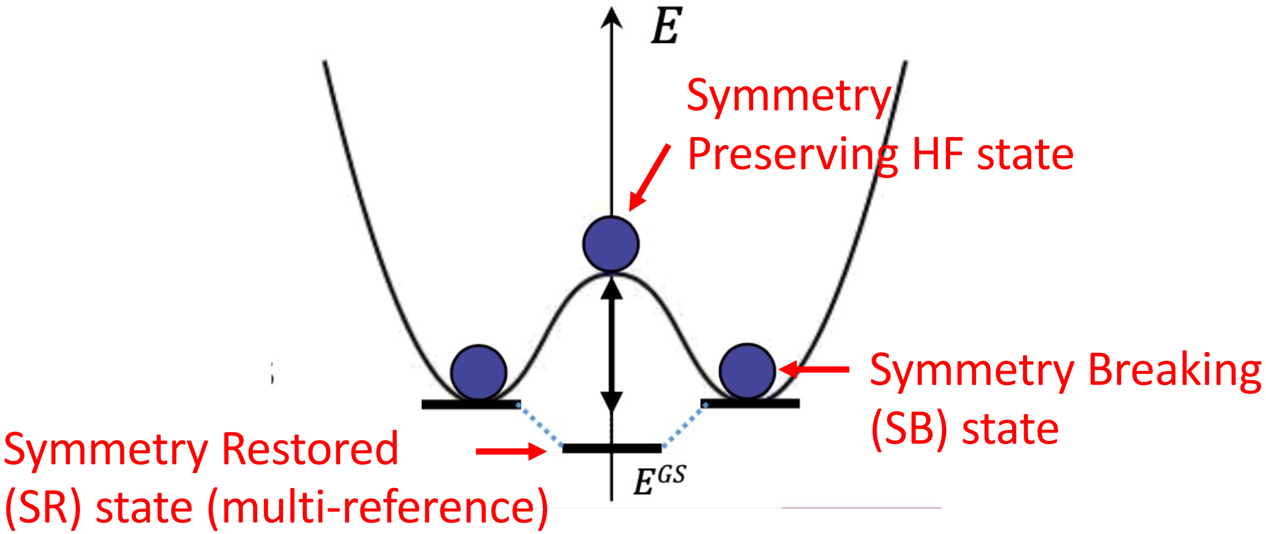
Illustration for small superfluids

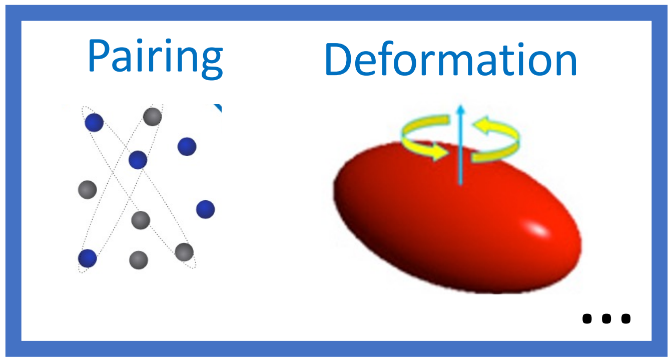


Example of mixing for 12 qubits



Restoring symmetries on a quantum computer?





D. Lacroix, A. Ruiz Guzman and P. Siwach,
Symmetry breaking/symmetry preserving circuits
and symmetry restoration on quantum computers
EPJA 59 (2023)

A brief overview of the symmetry restoration problem and its solution

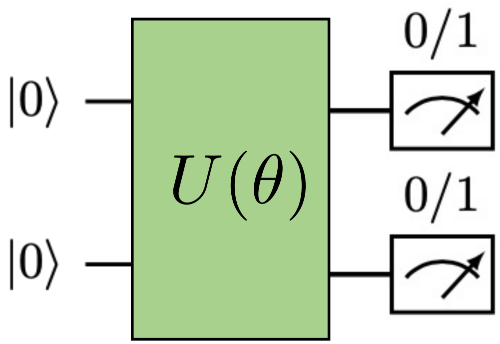
The particle number case

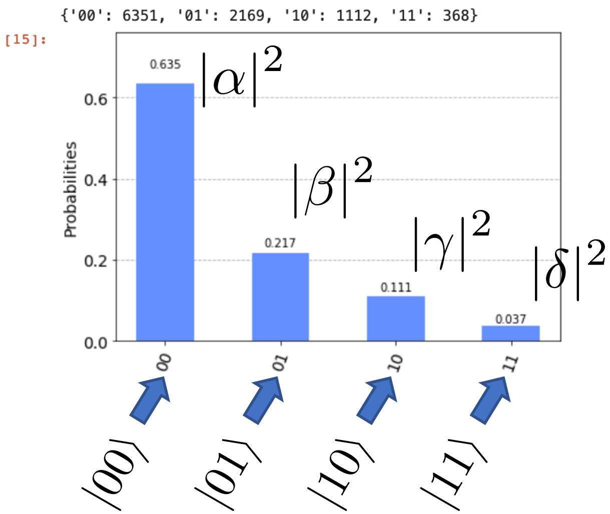
$$|\Psi\rangle = \sum_N c_N |N\rangle \Rightarrow |N\rangle \Rightarrow$$

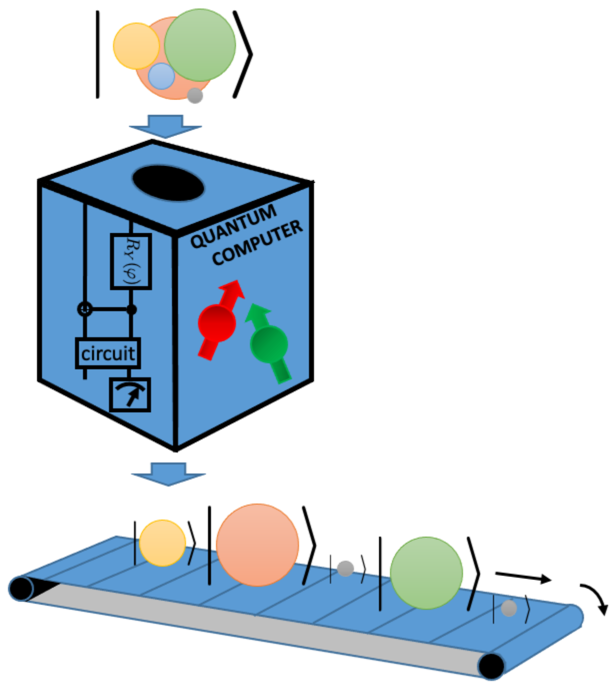
Use it for evolution,
Energy minimization, …

For 2 qubits

$$|\Psi\rangle = \underbrace{\alpha|00\rangle}_{|N=0\rangle} + \underbrace{\beta|01\rangle + \gamma|10\rangle}_{\propto |N=1\rangle} + \underbrace{\delta|11\rangle}_{|N=2\rangle}$$





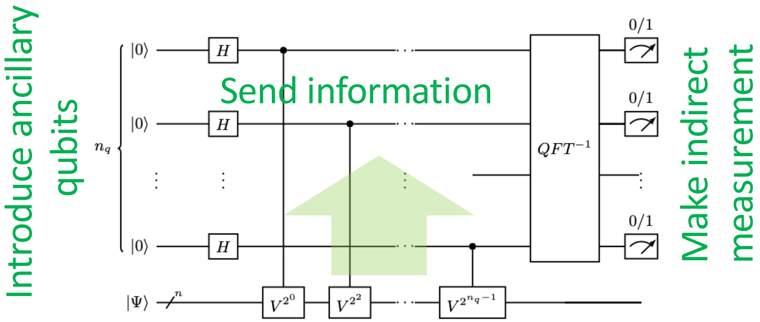


Difficulty – wave-function collapse

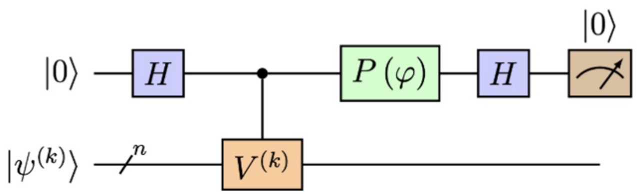
D. Lacroix, "*Symmetry-Assisted Preparation of Entangled Many-Body States on a Quantum Computer*", PRL 125, 230502 (2020).

Systematic of Symmetry filtering methods

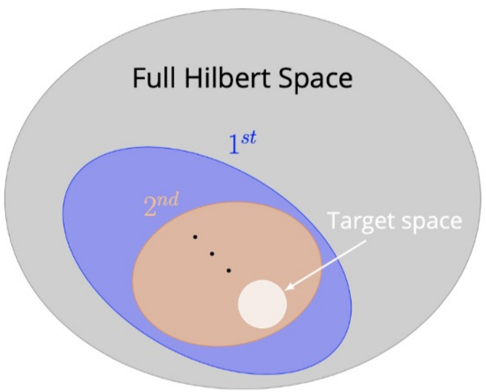
Standard Quantum Phase estimation



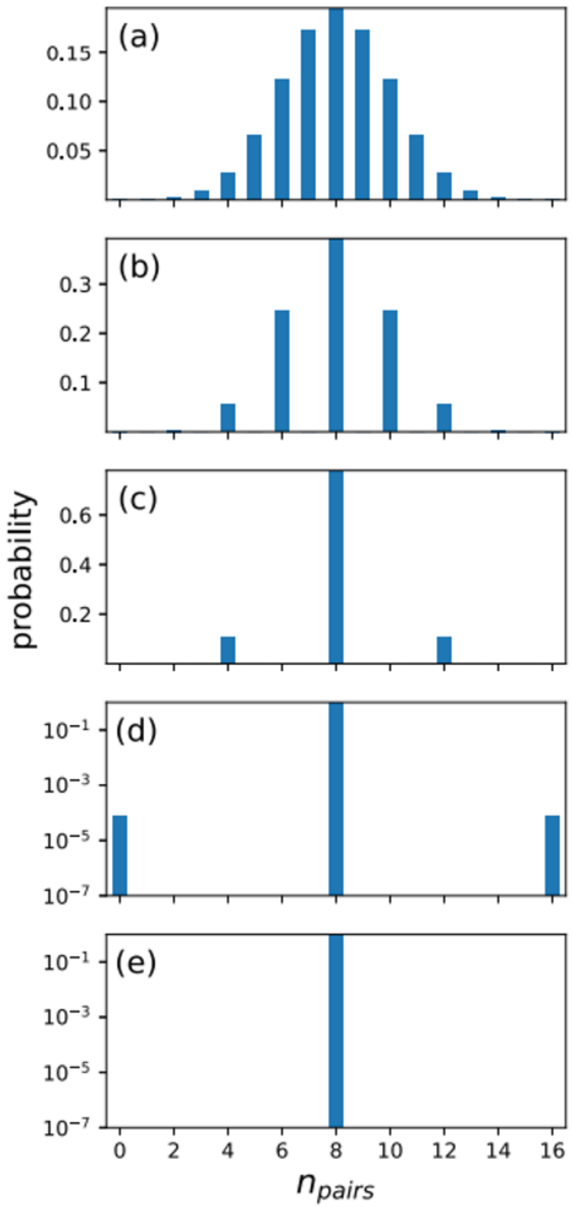
Iterative Quantum Phase estimation



$$\hat{V}^{(k)} = e^{i\phi_k \hat{N}} \qquad \phi_k = \frac{\pi}{2^k}$$



16 qubits, N = 8



D. Lacroix, Phys. Rev. Lett. 125 (2020).

1 Preparation of SB states on QC

2 Symmetry restoration on QC

3 Post-processing for Improved ground state or excited States (QPE, Quantum Krylov, …)

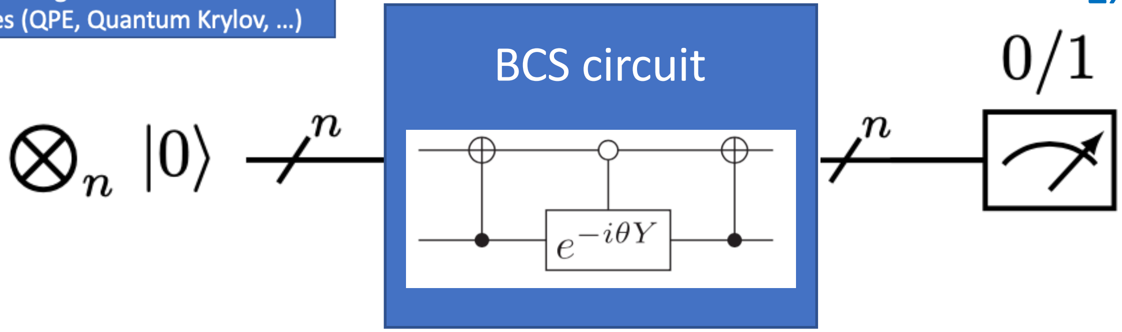
Standard nuclear physics strategy based on symmetries

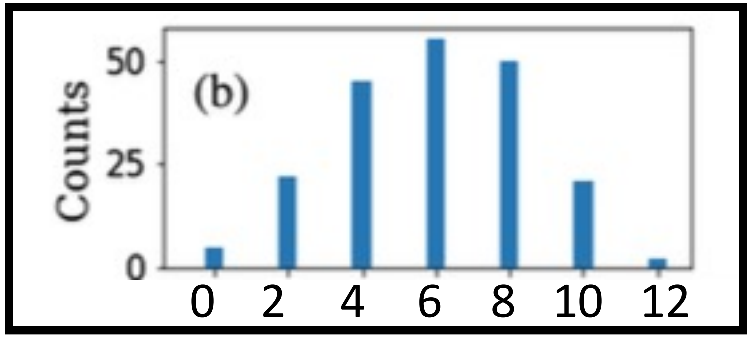
Where we are, where we go

1 Preparing symmetry-breaking state (BCS, …)

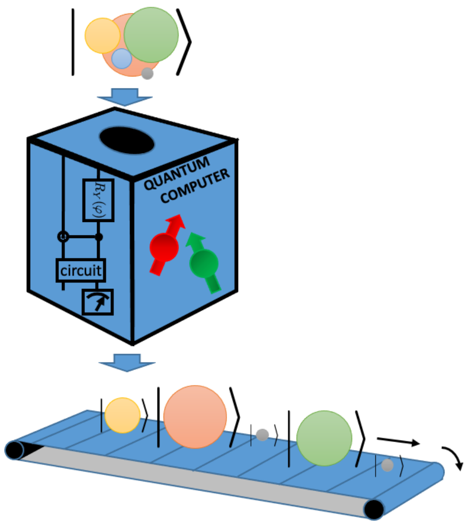
➡ Relatively easy, uses standard toolkit

Example of mixing for 12 qubits (with qiskit)





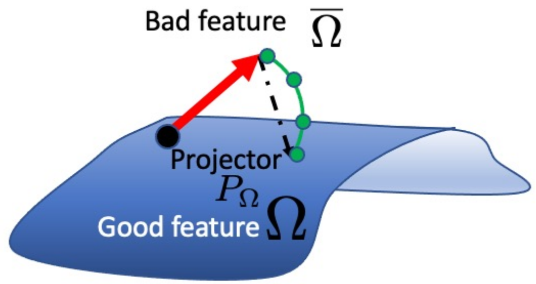
2 Restoring symmetries



Various methods

-With phase-estimation

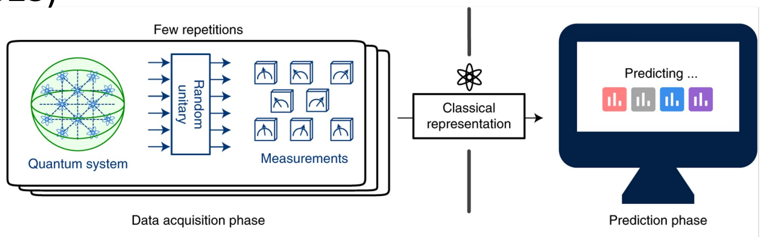
D. Lacroix, PRL 125, 230502 (2020).



-Using quantum Oracles

Ruiz Guzman, Lacroix, PRC 107 (2023)

-Using classical post-processing (shadows)



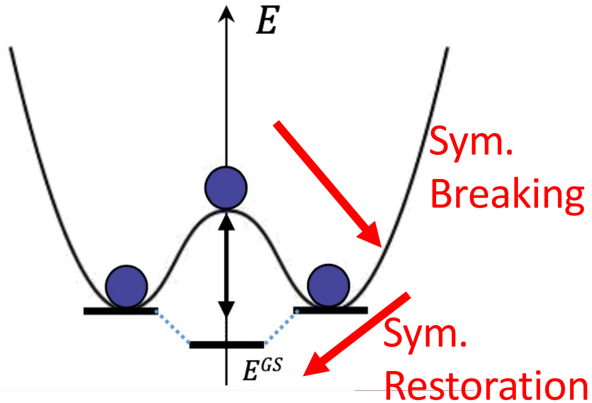
Ruiz Guzman, Lacroix, Eur. J. Phys. A 60 (2024)

Standard nuclear physics strategy based on symmetries

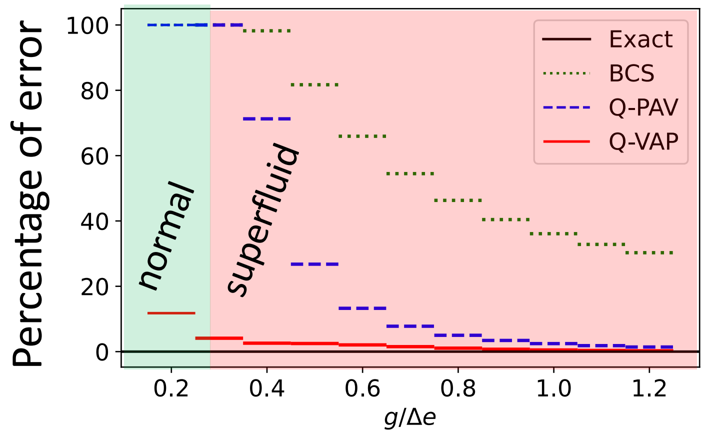
Where we are, where we go

1. Preparation of SB states on QC
2. Symmetry restoration on QC
3. Post-processing for Improved ground state or excited States (QPE, Quantum Krylov, …)

3 Using Symmetry-breaking / restoration



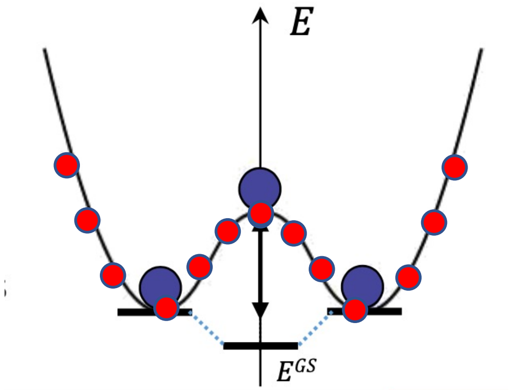
8 particles on 8 equidistant levels



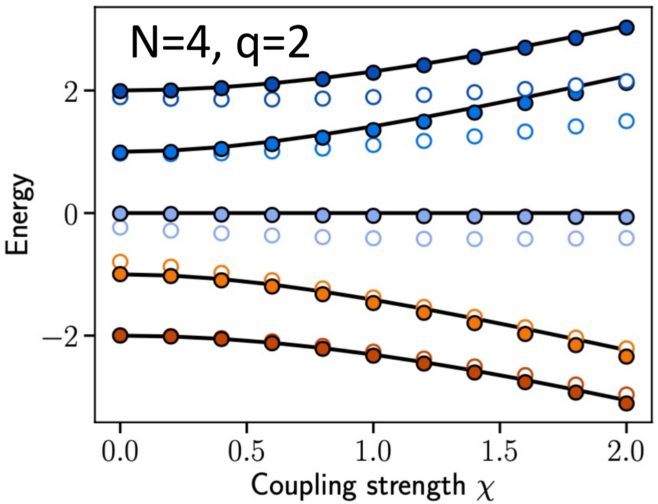
Quantum Generator Coordinate Method

$$|\Psi\rangle = \int_{\mathbf{q}} f(\mathbf{q}) |\Phi(\mathbf{q})\rangle d\mathbf{q}$$

$$\int_{\mathbf{q}'} d\mathbf{q}' \left[\mathcal{H}(\mathbf{q},\mathbf{q}') - E\mathcal{N}(\mathbf{q},\mathbf{q}')\right] f(\mathbf{q}') = 0$$

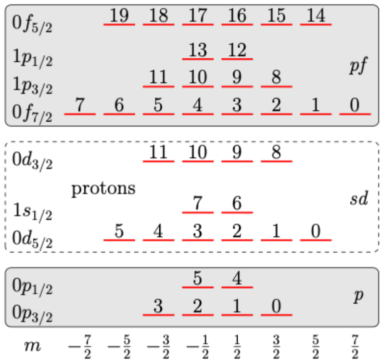


Lipkin model



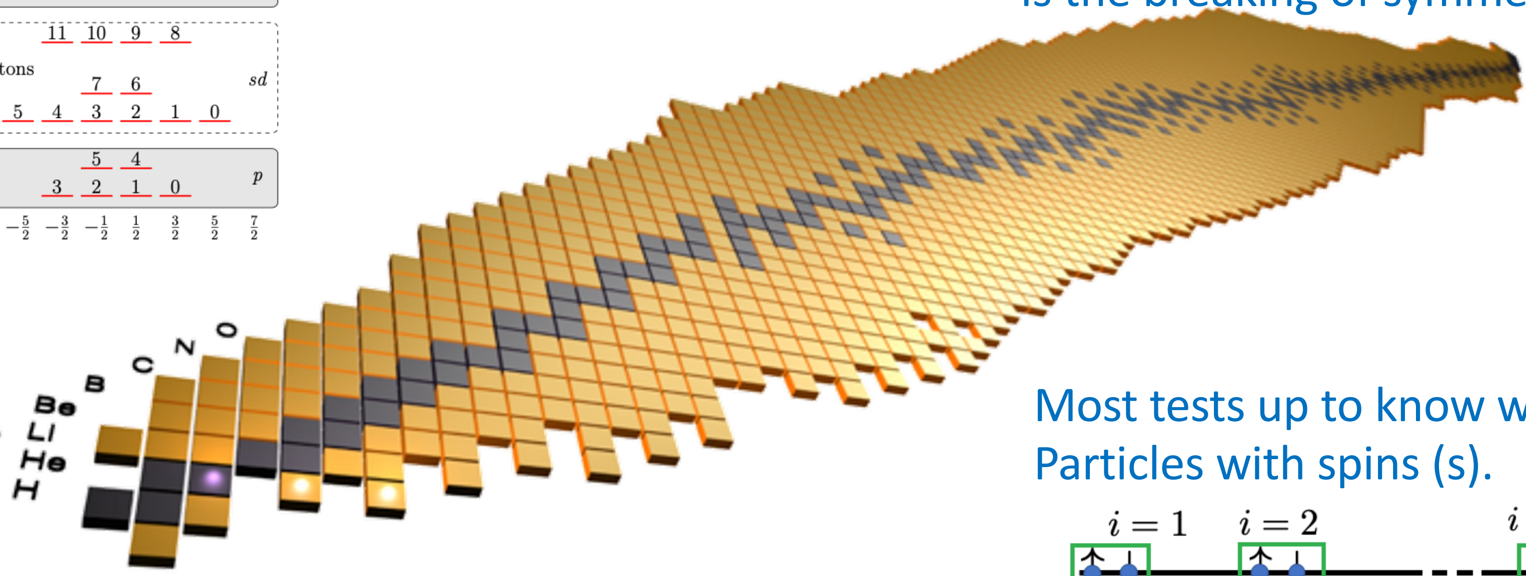
- Q-HFB
- Q-PAV
- Q-VAP
- Q-GCM

Beaujeault-Taudière, Lacroix, PRC 109 (2024)

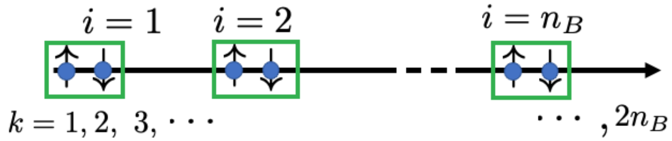


Getting closer to realistic problems

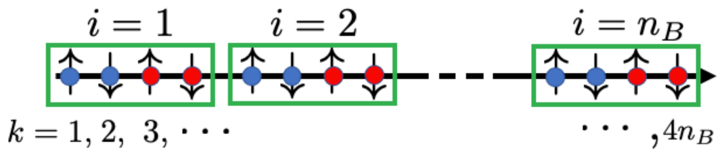
Is the breaking of symmetries always a good idea?



Most tests up to know were made on Particles with spins (s).



But nuclei have both spin (s) and isospin (t) (neutron/proton)



This increases the number of qubits

$$S_z, \ S^2, \ \pi$$

This increases the number of symmetries that could be broken

$$S_z, \ S^2, \ T_z, \ T^2, \ \pi$$

Symmetry-breaking states become extremely hard to control

Symmetry restoration becomes very demanding

J. Zhang, PhD thesis Paris-Saclay Univ. (2025).

Going beyond traditional nuclear physics methods: Use of adaptative methods

Iterative construction of the ansatz

Grimsley, et al, Nat. Commun. 10 (2019)

- Start from a state $|\Psi_0\rangle = |n=0\rangle$

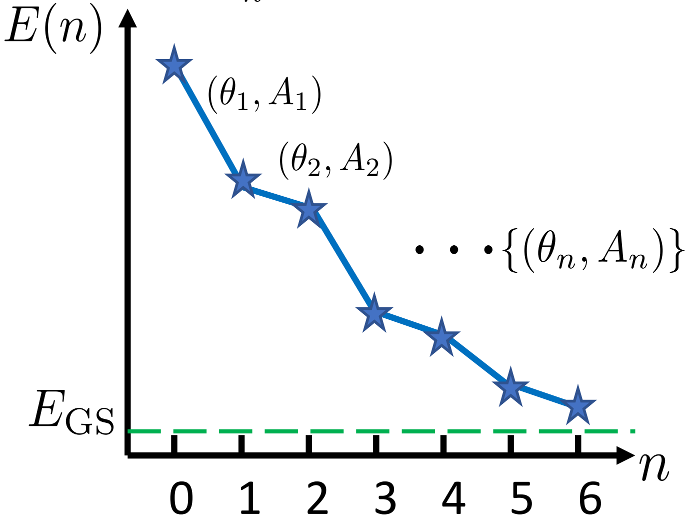
- Built iteratively the ansatz such as:

$$|n\rangle = e^{i\theta_n A_n}|n-1\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k}|0\rangle$$

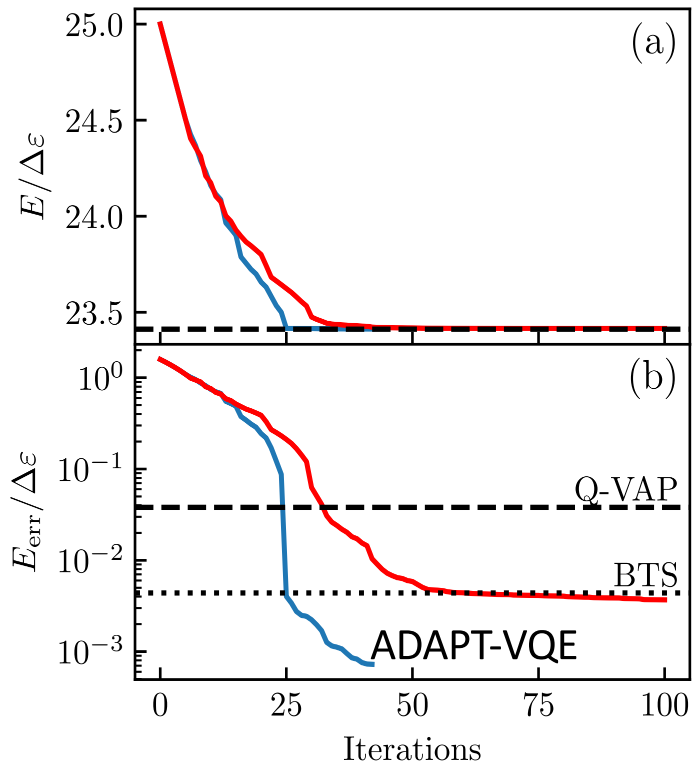
$$A_n \in \{O_1, \cdots, O_\Omega\}$$

Such that

$$\frac{\partial E(n)}{\partial \theta_n} = i\langle n|\,[H, A_n]\,|n\rangle$$ is maximum

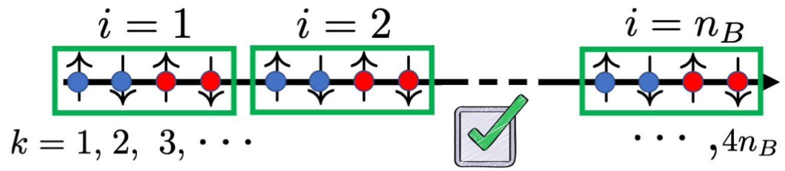


ADAPT-VQE applied to the Superfluid problems: only spins

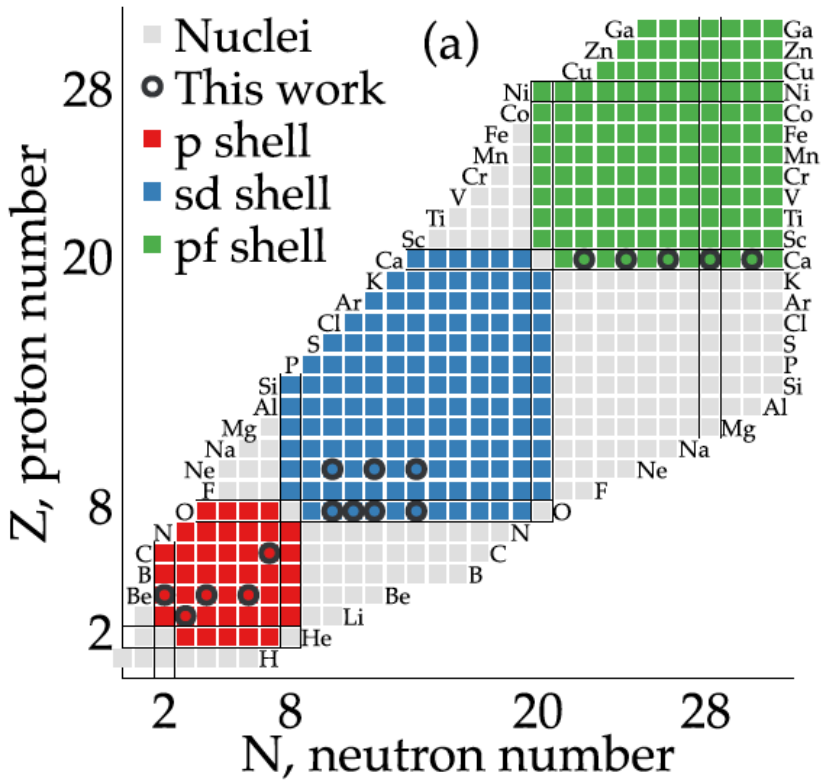


J. Zhang, D. Lacroix, and Y. Beaujeault-Taudière, PRC 110 (2024)

Extension to spin and isospin

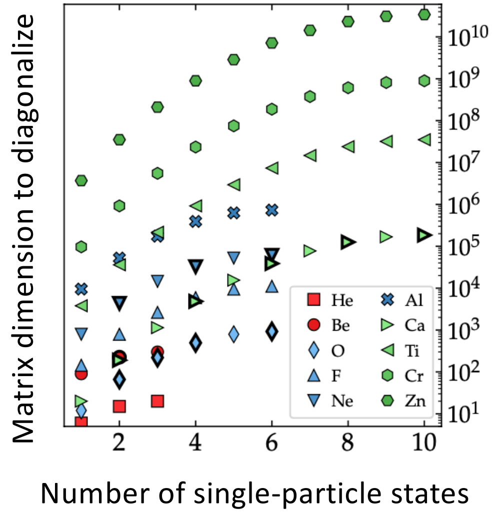


The nuclear shell model on quantum computers



Pérez-Obiol, et al
Scientific Reports 13, 12291 (2023)

Finding eigenstates



- Exponential growth of basis dimensions: $D \sim \binom{d_\pi}{p} \cdot \binom{d_\nu}{n}$

  In *pf* shell :
  ^{56}Ni **1,087,455,228**
  In *pf-sdg* space :
  ^{78}Ni **210,046,691,518**

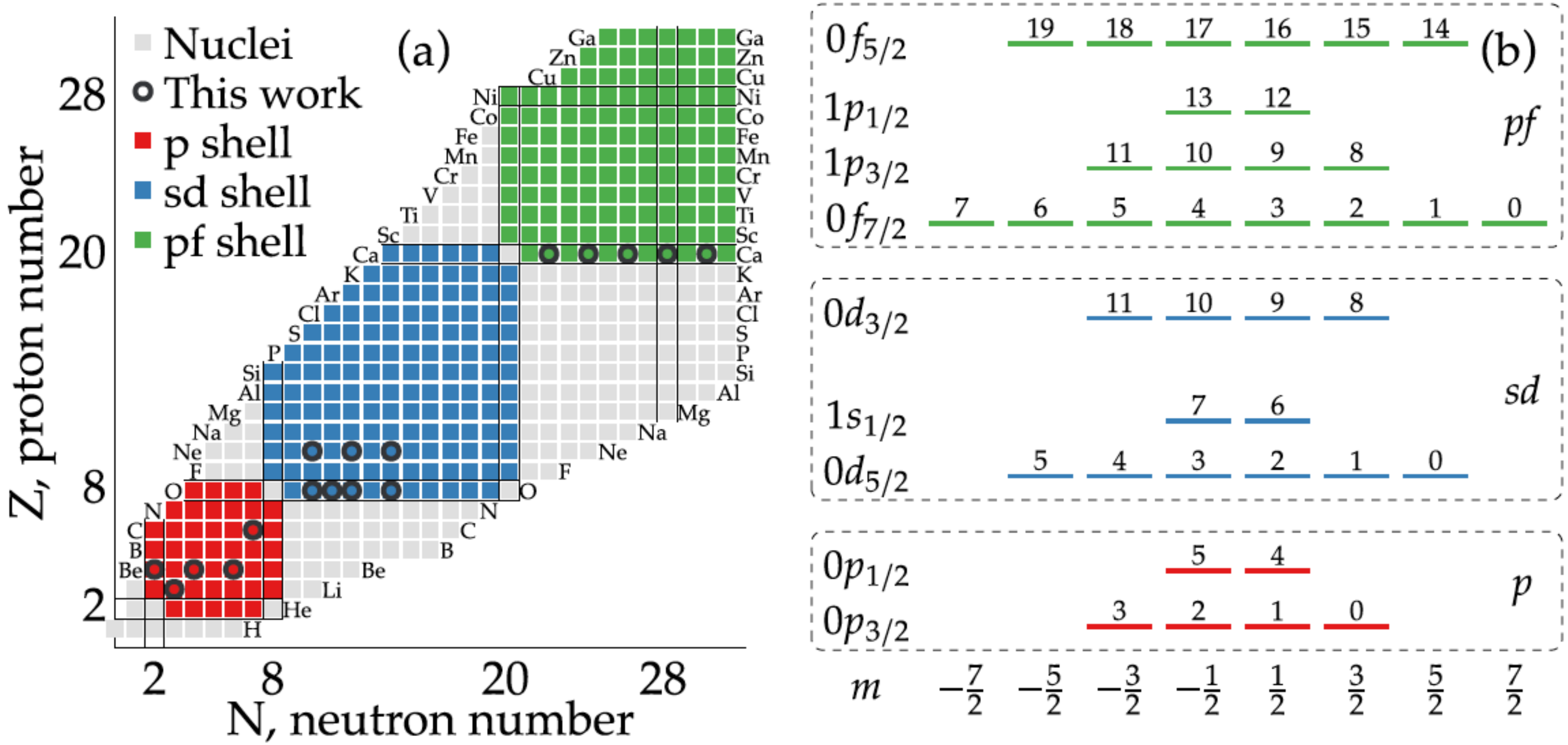
  $\simeq 30$ qubits
  $\simeq 38$ qubits

- Actual limits in giant diagonalizations: **0.2 10^{12}** (^{114}Sn)
- Largest matrices up to now: $\sim 10^{14}$ non-zero matrix elements
- Strasbourg LSSM codes: **ANTOINE** and **NATHAN**

(courtesy F. Nowacki [2021])

The nuclear shell model on quantum computers

Valence space quantum computing



20 or less qubits

Obiol et al, 2302.03641
Bhoy et al, 2402.15577
Costa et al, 2411.06954
Yoshida et al, 2404.01694
Yoshida et al, 2509.20642
…

12 or less qubits

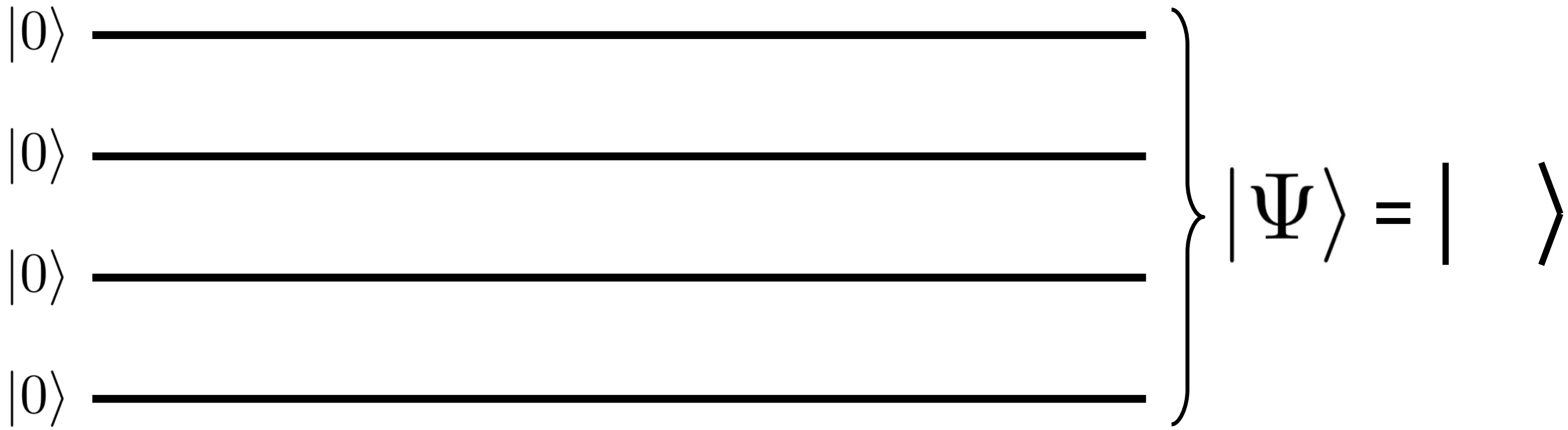
Sarma et al, 2306.06432
Yang et al, 2306.08885
Sarma et al, 2510.02124
…

6 or less qubits

Carrasco-Codina et al, 2507.13819
…

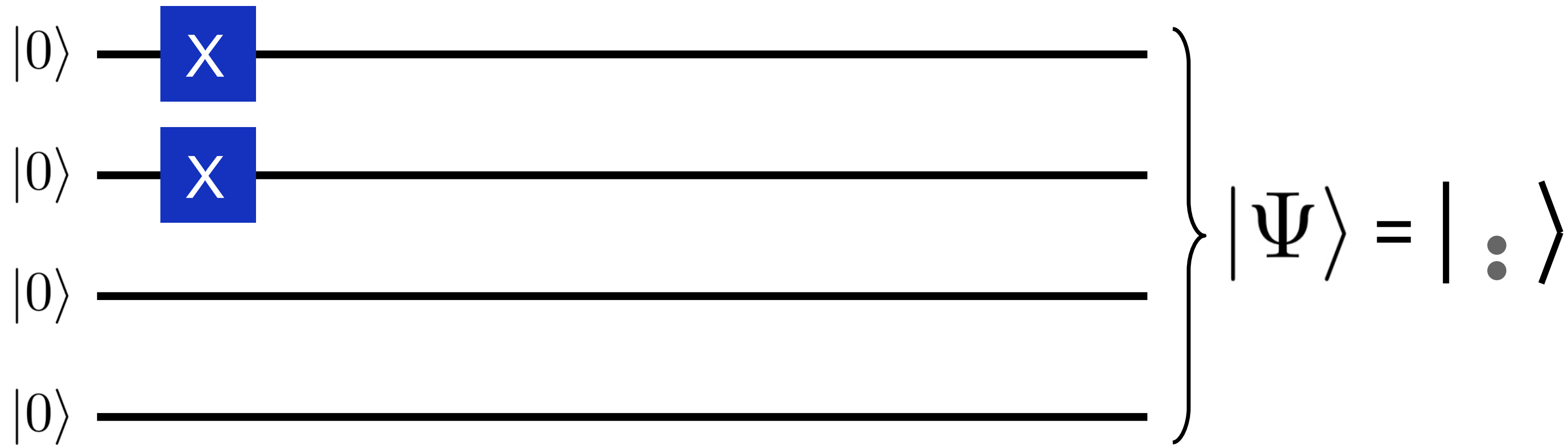
- Select the model space
- Fermion-to-qubit mapping
- Use your favorite variational technique

Qubits provide an efficient representation of a many-body wavefunction



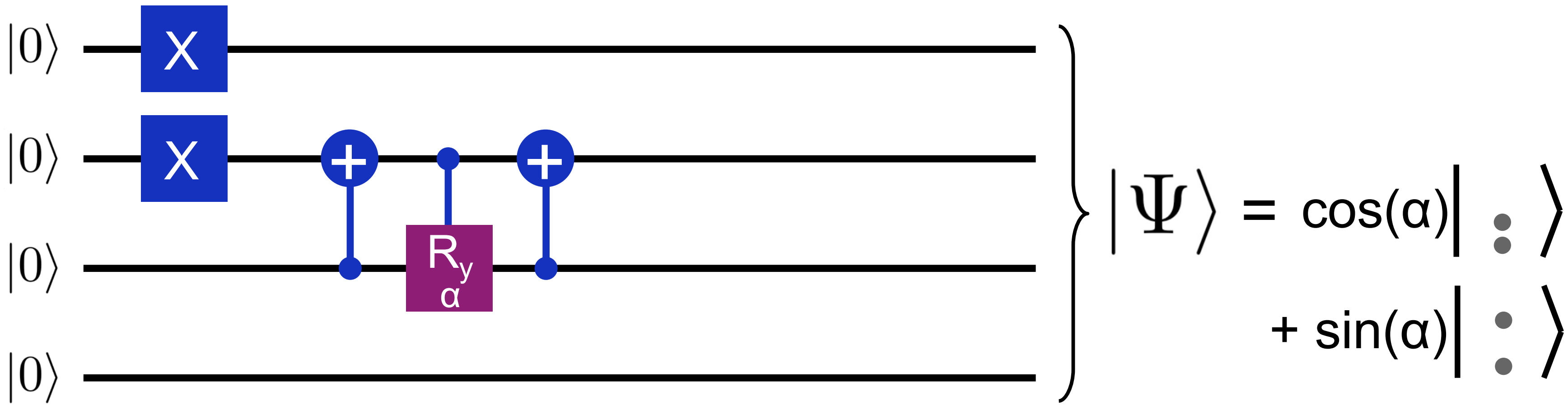
(courtesy S. Aychet-Claisse [PhD IJCLab/CEA Saclay])

Qubits provide an efficient representation of a many-body wavefunction



(courtesy S. Aychet-Claisse [PhD IJCLab/CEA Saclay])

Qubits provide an efficient representation of a many-body wavefunction



(courtesy S. Aychet-Claisse [PhD IJCLab/CEA Saclay])

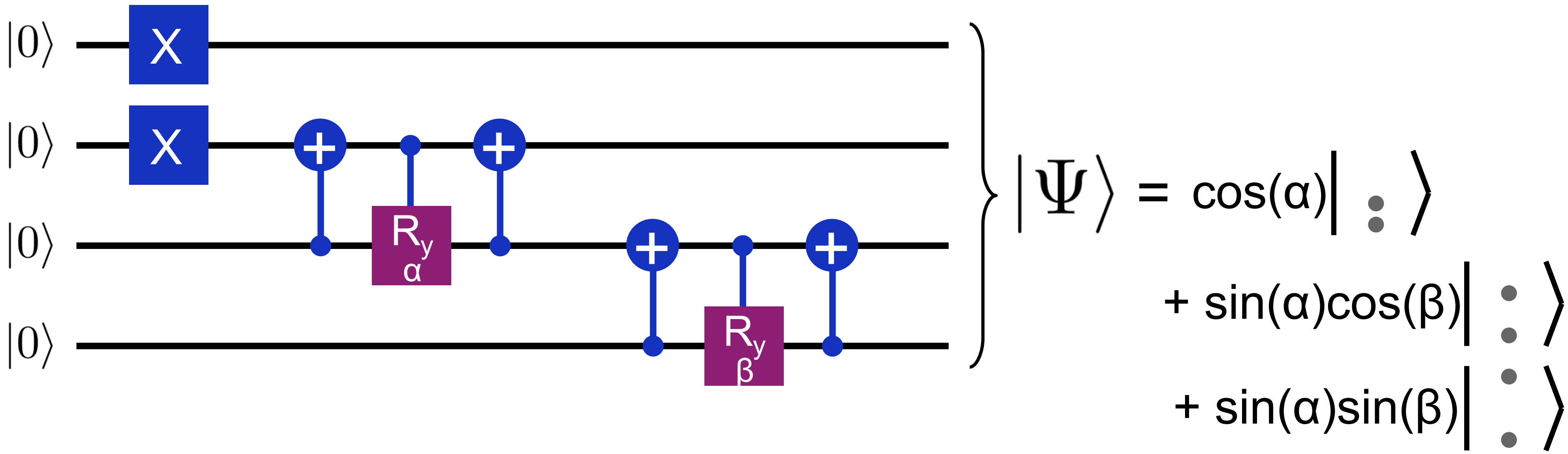
Qubits provide an efficient representation of a many-body wavefunction

$$
\begin{array}{cccc}
|00\rangle & |01\rangle & |10\rangle & |11\rangle \\
\end{array}
$$
$$
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos(\alpha) & -\sin(\alpha) & 0 \\
0 & \sin(\alpha) & \cos(\alpha) & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
$$

Creates entanglement between qubits

(courtesy S. Aychet-Claisse [PhD IJCLab/CEA Saclay])

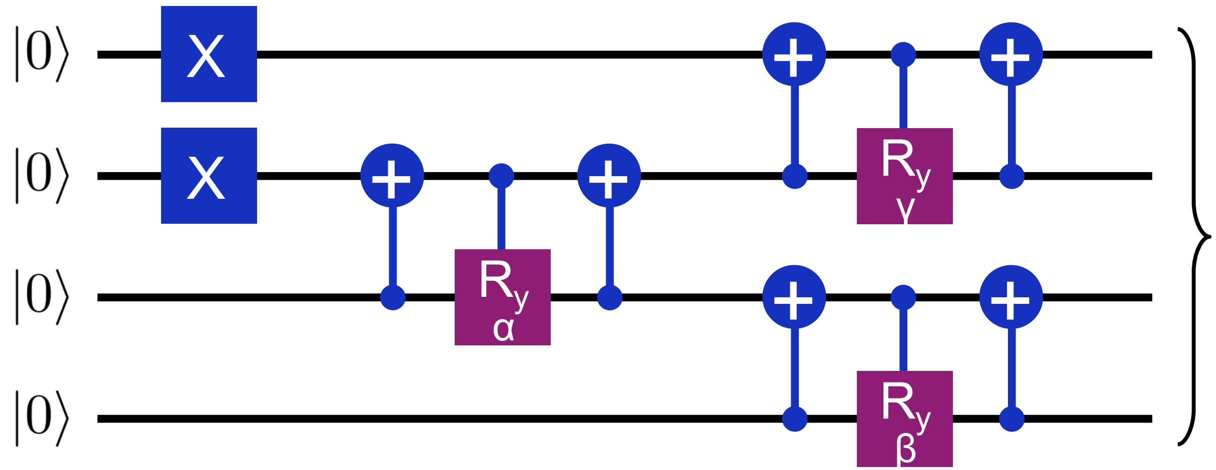
Qubits provide an efficient representation of a many-body wavefunction

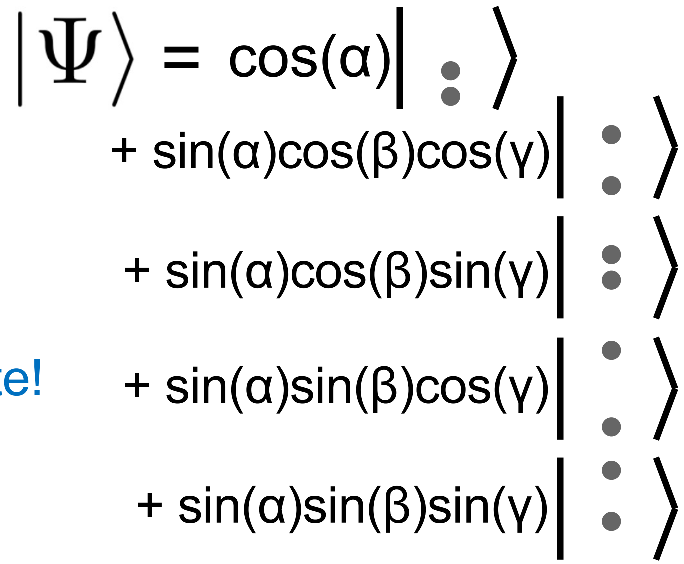


(courtesy S. Aychet-Claisse [PhD IJCLab/CEA Saclay])

Building a state

Qubits provide an efficient representation of a many-body wavefunction





n qubits are sufficient to represent a n-level many-body state!
The Hilbert space has 2^n states

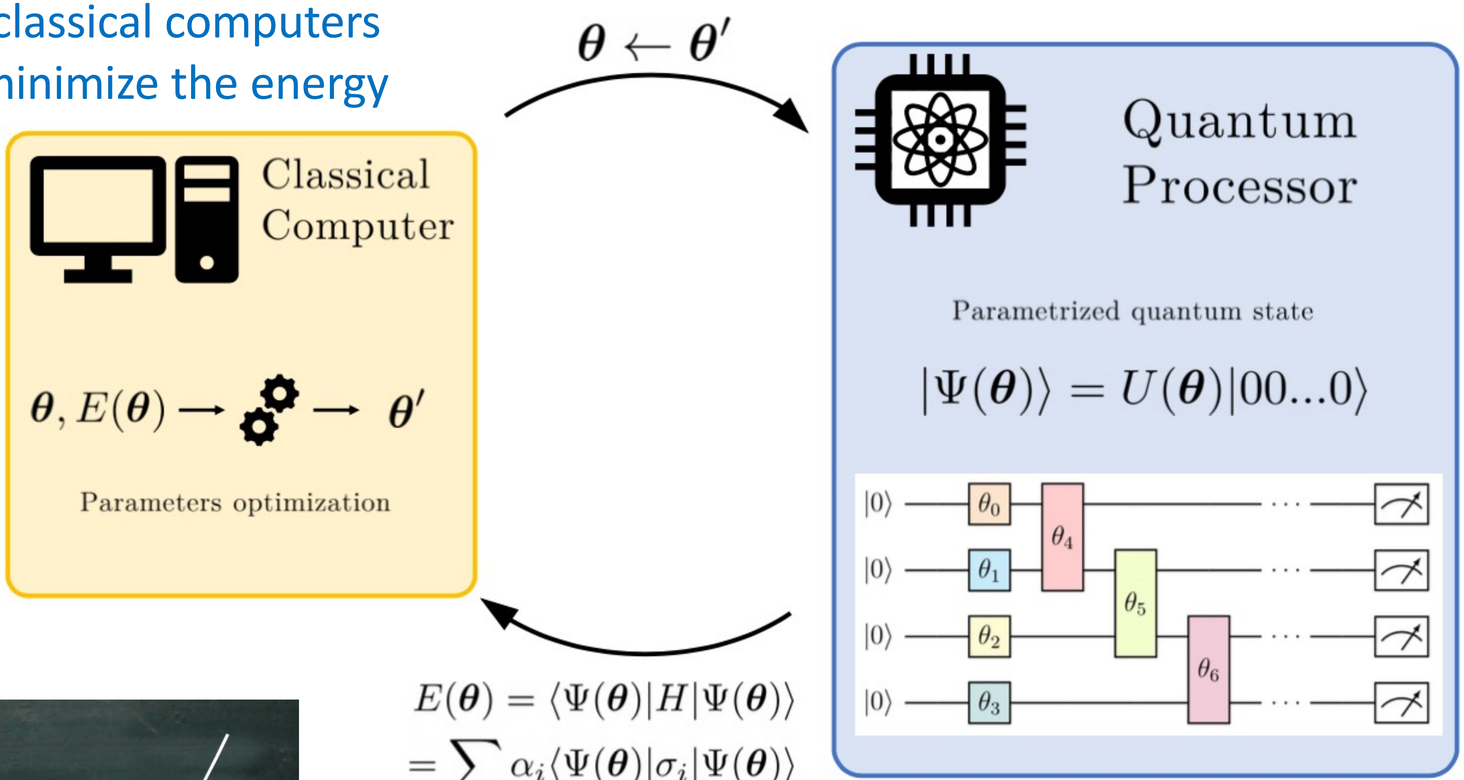
Today's advanced shell model calculations are able to treat matrices of the order of 100 million states.
30 qubits allow for treating matrices of 1 billion states!

(courtesy S. Aychet-Claisse [PhD IJCLab/CEA Saclay])

Preparing quantum ansatz and Variational Quantum Eigensolver methods

1 The state is prepared on the quantum computer

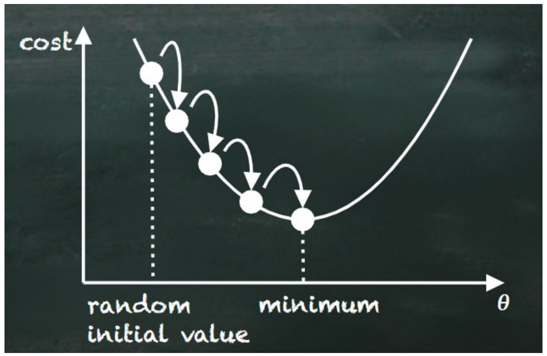
3 The parameters are optimized in classical computers to minimize the energy



$$E(\boldsymbol{\theta}) = \langle\Psi(\boldsymbol{\theta})|H|\Psi(\boldsymbol{\theta})\rangle$$
$$= \sum_i \alpha_i \langle\Psi(\boldsymbol{\theta})|\sigma_i|\Psi(\boldsymbol{\theta})\rangle$$

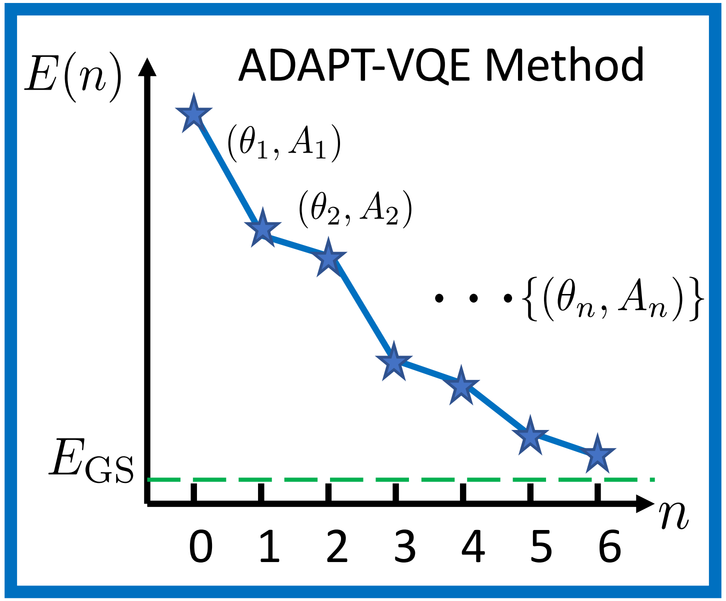
Anselme-Martin, PhD Thesis, Univ. Paris-Saclay

2 The energy of the state is built from the measurements made on the system



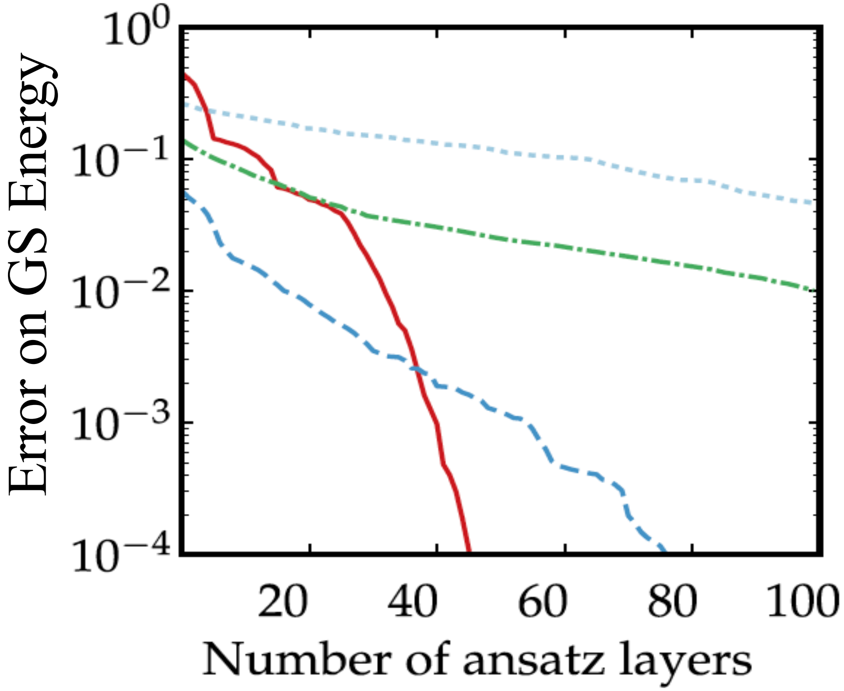
Today's applications

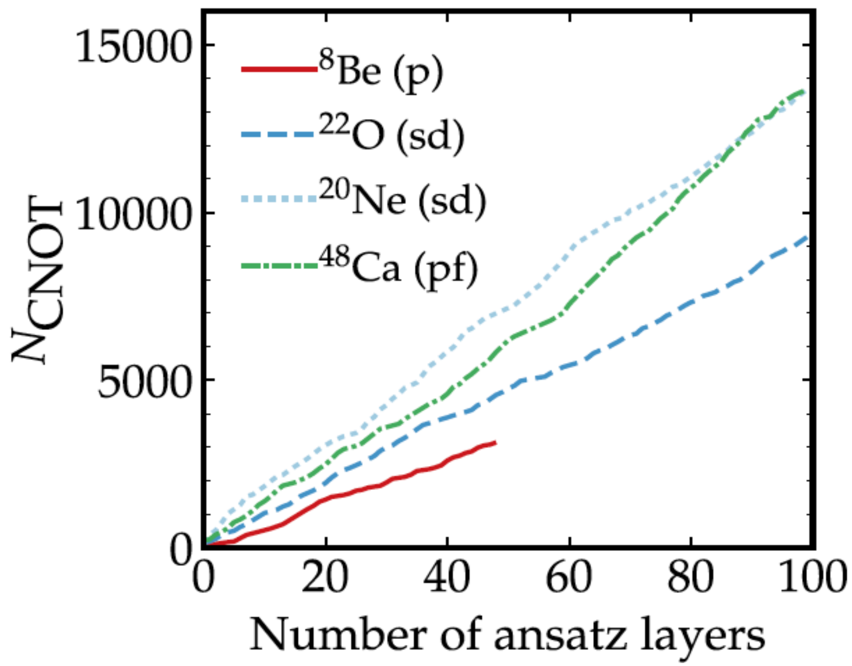
Illustration of Shell Model applications



Pool operator inspired from Coupled-Cluster

$$
\begin{cases}
A^{(1)}_{ij} \equiv (Q^+_i Q_j - Q^+_j Q_i) = \frac{i}{2}(X_i Y_j - Y_i X_j), & \text{single} \\
A^{(2)}_{ijkl} \equiv Q^+_i Q^+_j Q_k Q_l - Q^+_l Q^+_k Q_j Q_i & \text{double} \\
\quad = \frac{i}{8}(X_i Y_j X_k X_l + Y_i X_j X_k X_l & \\
\quad + Y_i Y_j Y_k X_l + Y_i Y_j X_k Y_l - X_i X_j Y_k X_l & \\
\quad - X_i X_j X_k Y_l - Y_i X_j Y_k Y_l - X_i Y_j Y_k Y_l). &
\end{cases}
$$

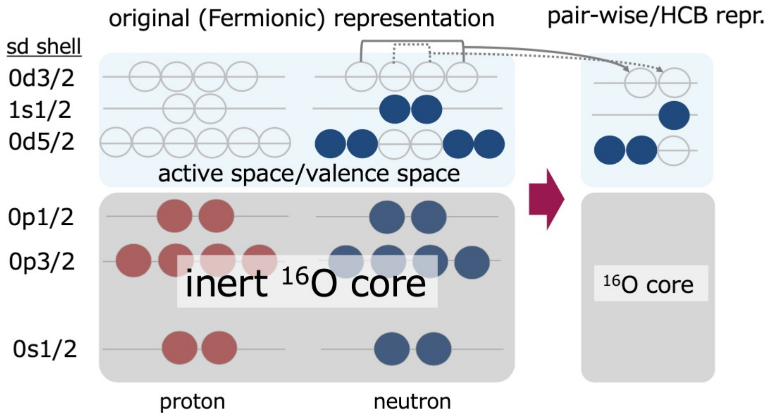


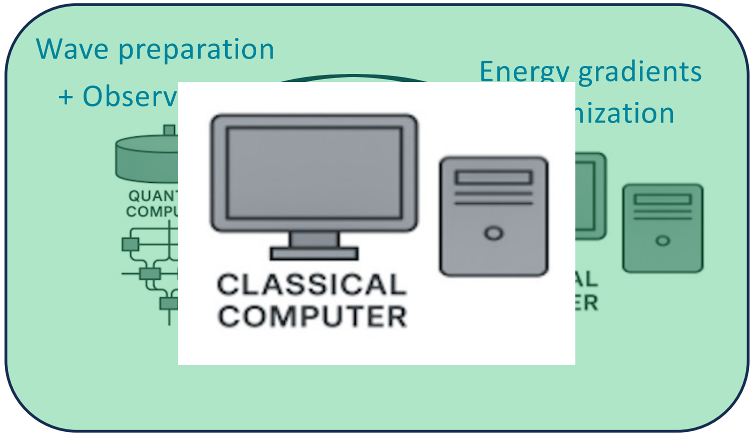


Pérez-Obiol, et al, Scientific Reports 13, 12291 (2023)

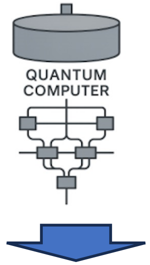
Simplified Shell Model applications on real quantum computers

Hard-core Boson mapping





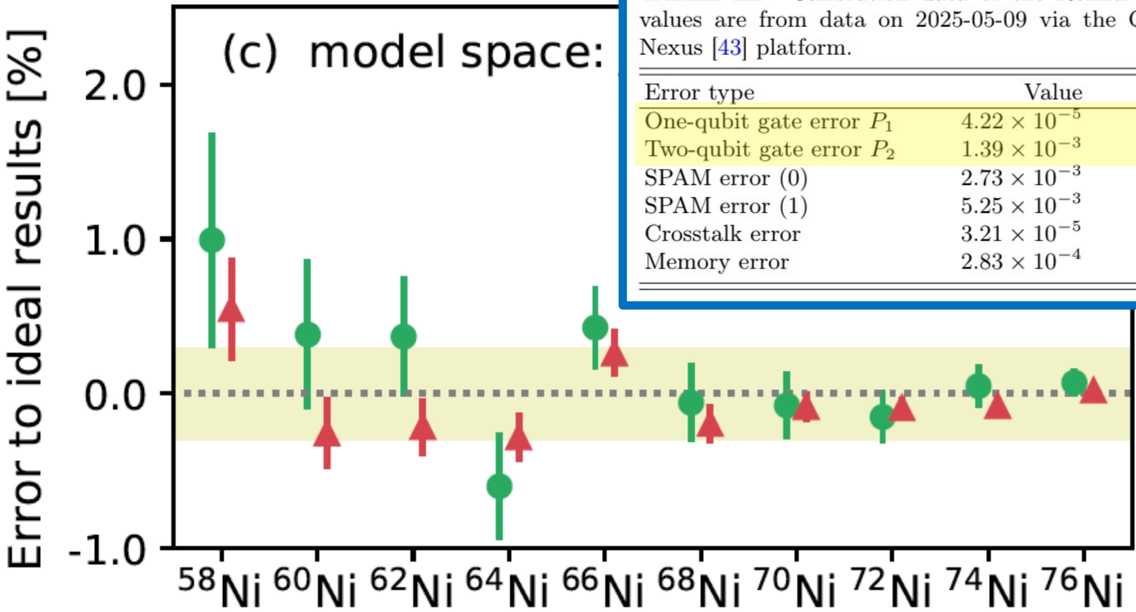
After optimal
solution
Is found



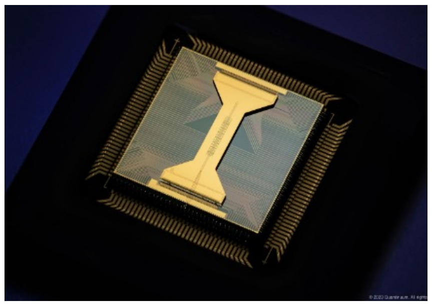
Build the
Approximate GS
Compute observable

TABLE III. Calibration data of the Reimei device. The values are from data on 2025-05-09 via the Quantinuum's Nexus [43] platform.

Error type	Value	Uncertainty
One-qubit gate error P_1	4.22×10^{-5}	5.23×10^{-6}
Two-qubit gate error P_2	1.39×10^{-3}	5.92×10^{-5}
SPAM error (0)	2.73×10^{-3}	1.57×10^{-4}
SPAM error (1)	5.25×10^{-3}	2.18×10^{-4}
Crosstalk error	3.21×10^{-5}	1.89×10^{-6}
Memory error	2.83×10^{-4}	2.32×10^{-5}

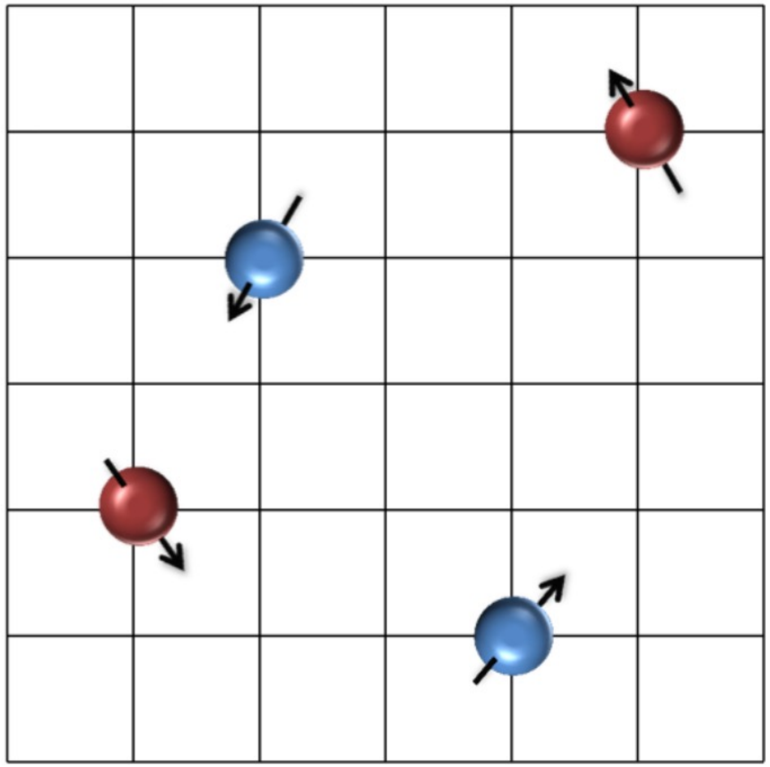


RIKEN-Quantinuum's
Reimei device
(trapped Ion)



Sota Yoshida, Takeshi Sato, Takumi Ogata, Masaaki Kimura, Phys. Rev. Res. (2026)

Quantum simulation of nuclei on lattices

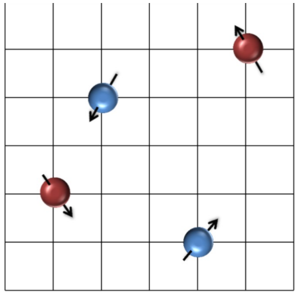


Dean Lee, Prog. Part. Nucl. Phys. (2009)
Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer

(courtesy T. Papenbrock)

Today's applications

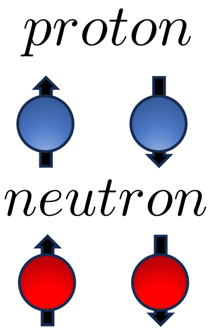
Quantum simulation of nuclei on lattices

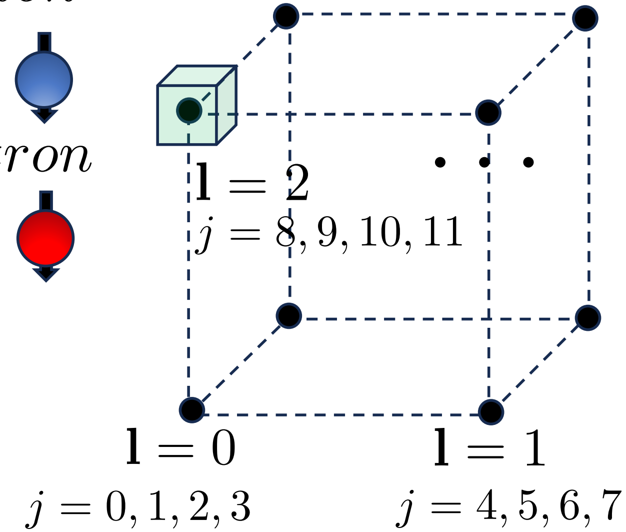


$L \times L \times L$ lattice

(here $L = 2$)

Number of single-particle states: $4L^3$





Pionless EFT Hamiltonian [Bedaque, van Kolck 2002]

$$\hat{H} = \sum_{\langle \mathbf{l},\mathbf{l}' \rangle} \sum_{\tau s} T^{\mathbf{l}}_{\mathbf{l}'} \hat{a}^{\dagger}_{\mathbf{l}\tau s} \hat{a}_{\mathbf{l}'\tau s}$$ Kinetic-non local

$$+ \frac{V}{2} \sum_{\mathbf{l}} \sum_{ss'\tau\tau'} \hat{a}^{\dagger}_{\mathbf{l}\tau s} \hat{a}^{\dagger}_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau s}$$ Two-body local

$$+ W \sum_{\mathbf{l}} \sum_{\tau s} \hat{a}^{\dagger}_{\mathbf{l}\tau\uparrow} \hat{a}^{\dagger}_{\mathbf{l}\tau\downarrow} \hat{a}^{\dagger}_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}\tau\downarrow} \hat{a}_{\mathbf{l}\tau\uparrow} .$$ Three-body local

Fermion to qubit mapping

$$\hat{H}_2(\mathbf{l}) = \frac{V}{4} \sum_{\alpha<\beta} (1 - Z_{\mathbf{l},\alpha})\,(1 - Z_{\mathbf{l},\beta})$$

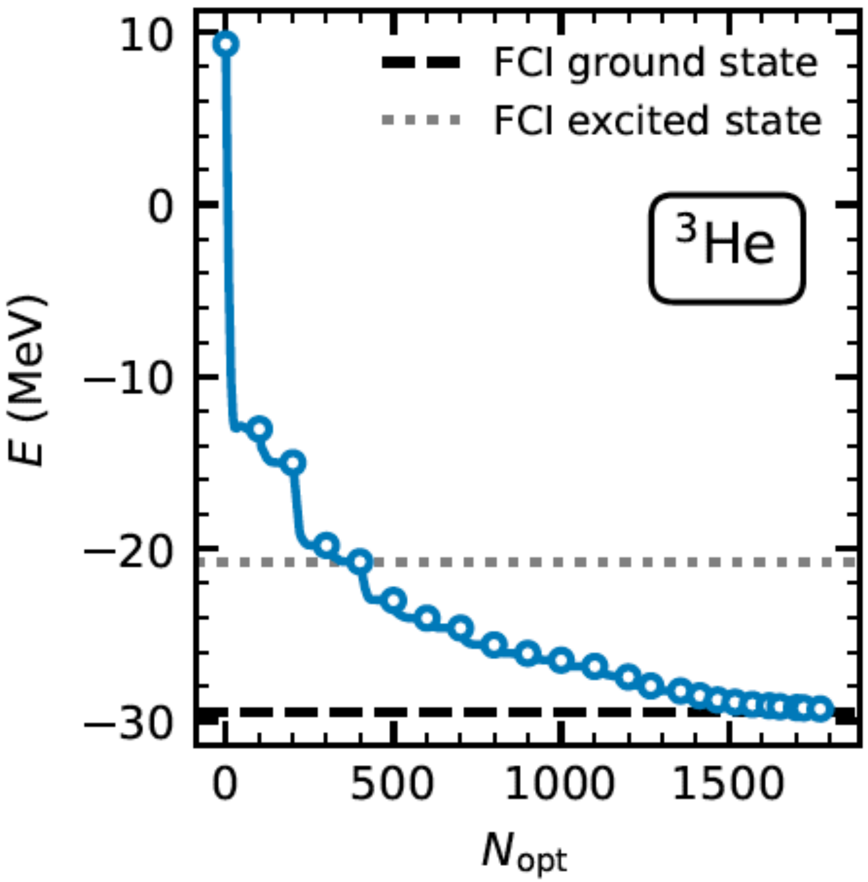
$$\hat{H}_3(\mathbf{l}) = \frac{W}{8} \sum_{\alpha<\beta<\gamma} (1 - Z_{\mathbf{l},\alpha})(1 - Z_{\mathbf{l},\beta})(1 - Z_{\mathbf{l},\gamma}).$$

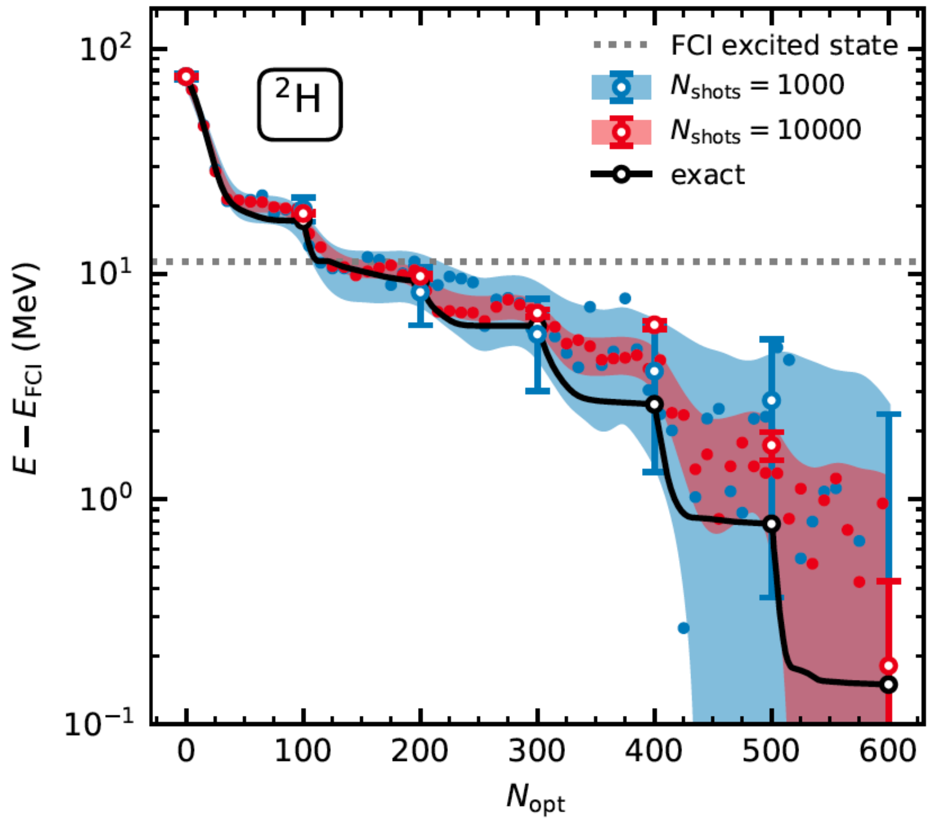
But…

$$\hat{H}_{\mathrm{kin}} = \sum_j T_{jj} \frac{1 - Z_j}{2} + \sum_{j<k} \frac{T_{jk}}{2} \left(X_j Z_{j+1} \cdots Z_{k-1} X_k + Y_j Z_{j+1} \cdots Z_{k-1} Y_k \right)$$

Application of ^{2}H and ^{3}He on a 2×2×2 lattice

$$|\vec{\theta}\rangle = \prod_{\alpha=1}^{N_e} \exp\left(\sum_{\beta=1}^{N_p} \theta_{\alpha\beta}\hat{A}_{\alpha\beta}\right)|\phi_0\rangle$$



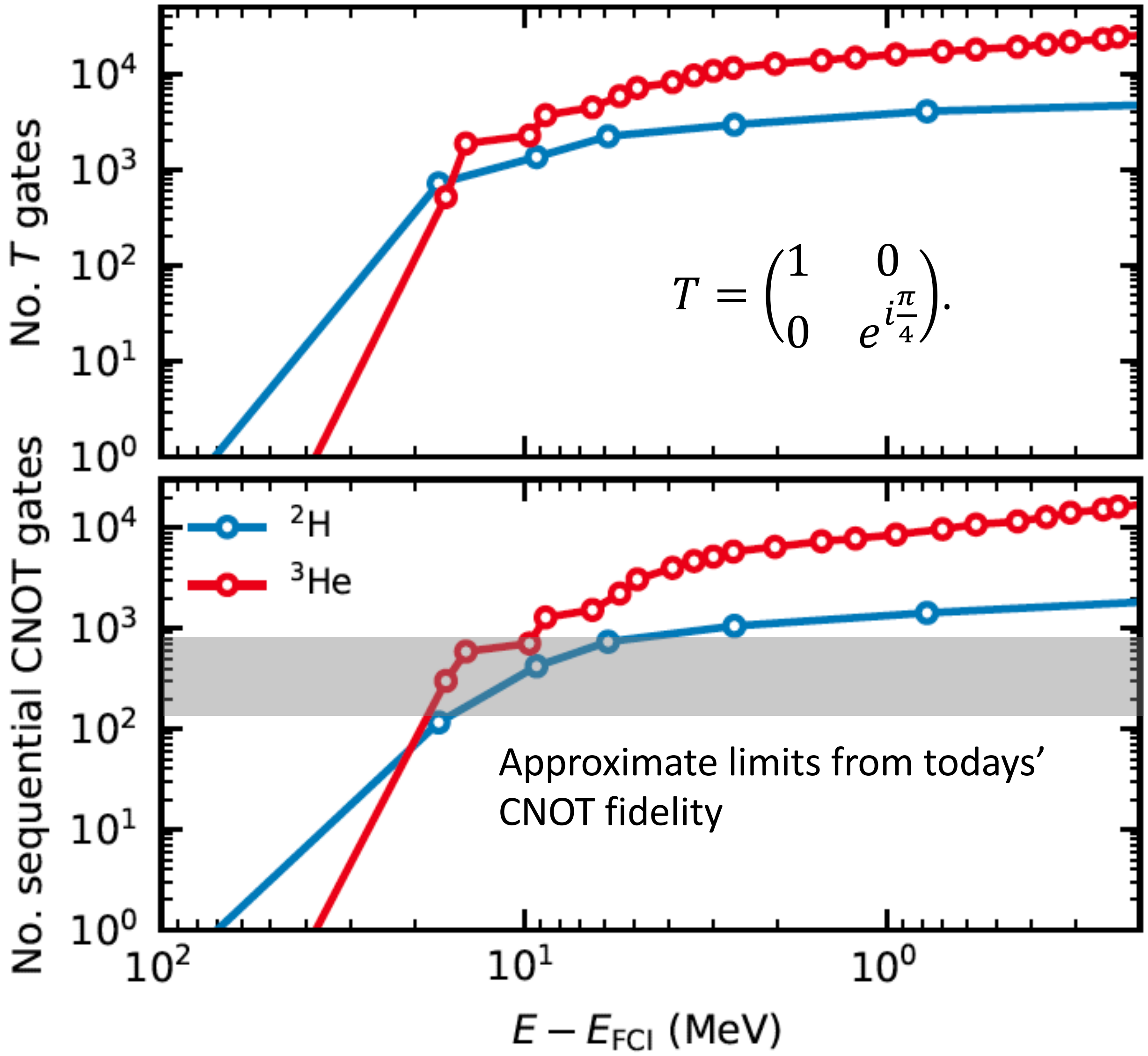


Gu, Heinz, Kiss, Papenbrock, Phys. Rev. C 113 (2026)

Application of 2H and 3He on a 2×2×2 lattice

Circuit complexity

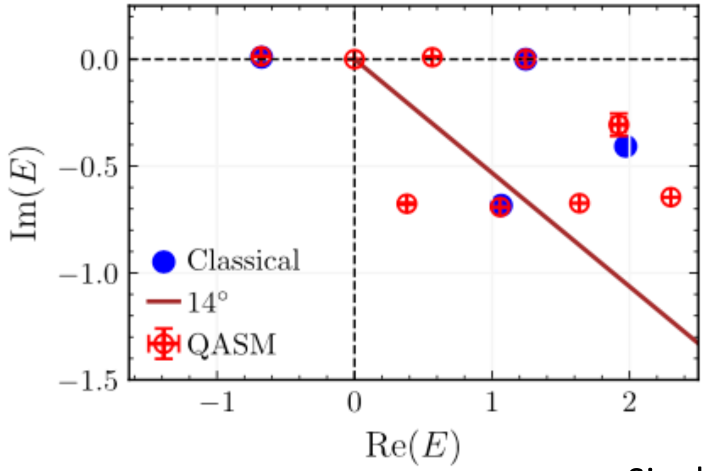
Gu, Heinz, Kiss, Papenbrock, Phys. Rev. C 113 (2026)



(courtesy T. Papenbrock)

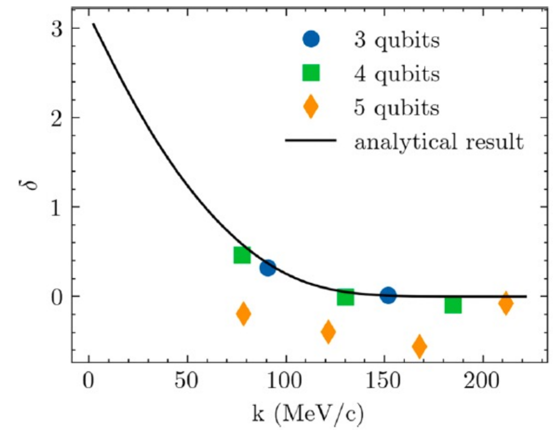
Other ongoing developments

Extraction of resonances (complex energy)



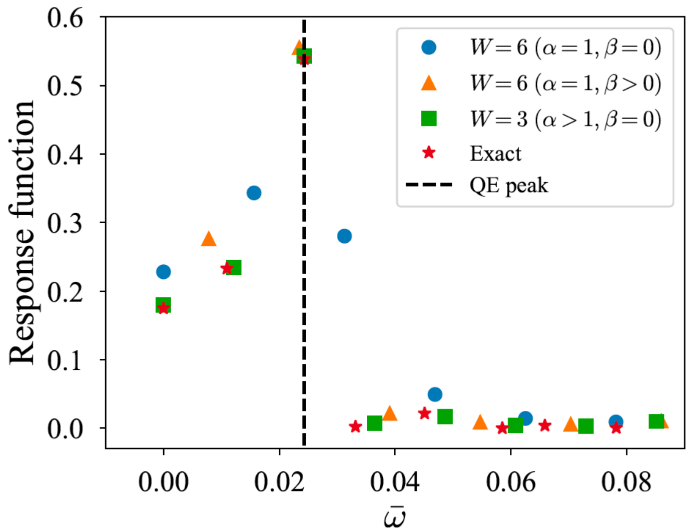
Singh et al (2025)

Phase-shift on quantum computers



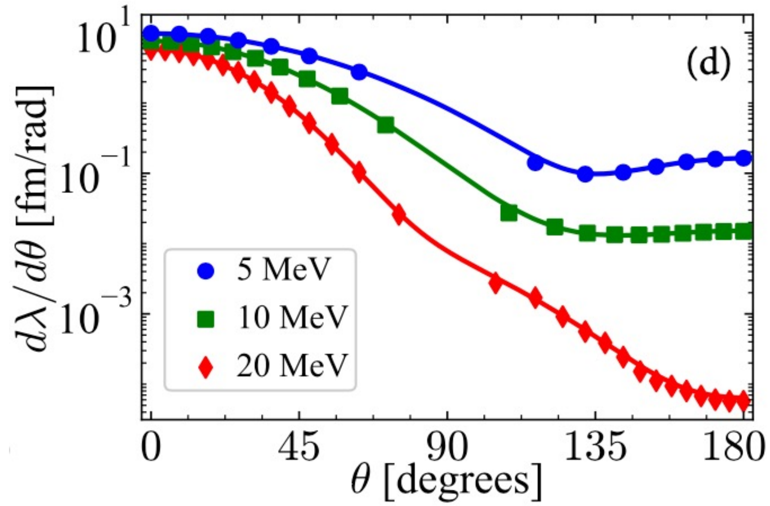
Sharma et al (2023); Wang et al (2024)

Response function



Weiss, et al (2025); Roggero et al (2019)

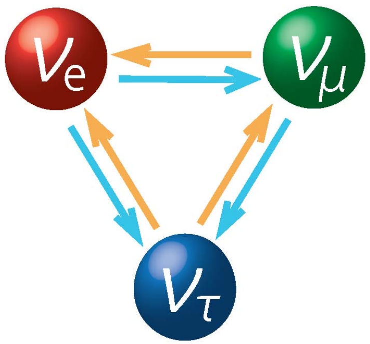
Nuclear reactions

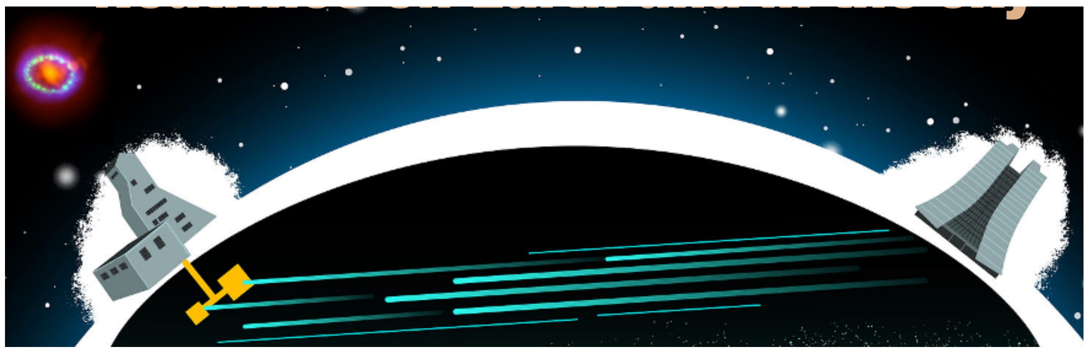


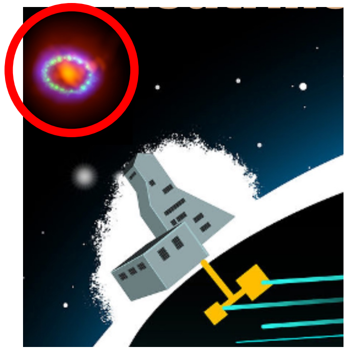
Rule et al (2025)

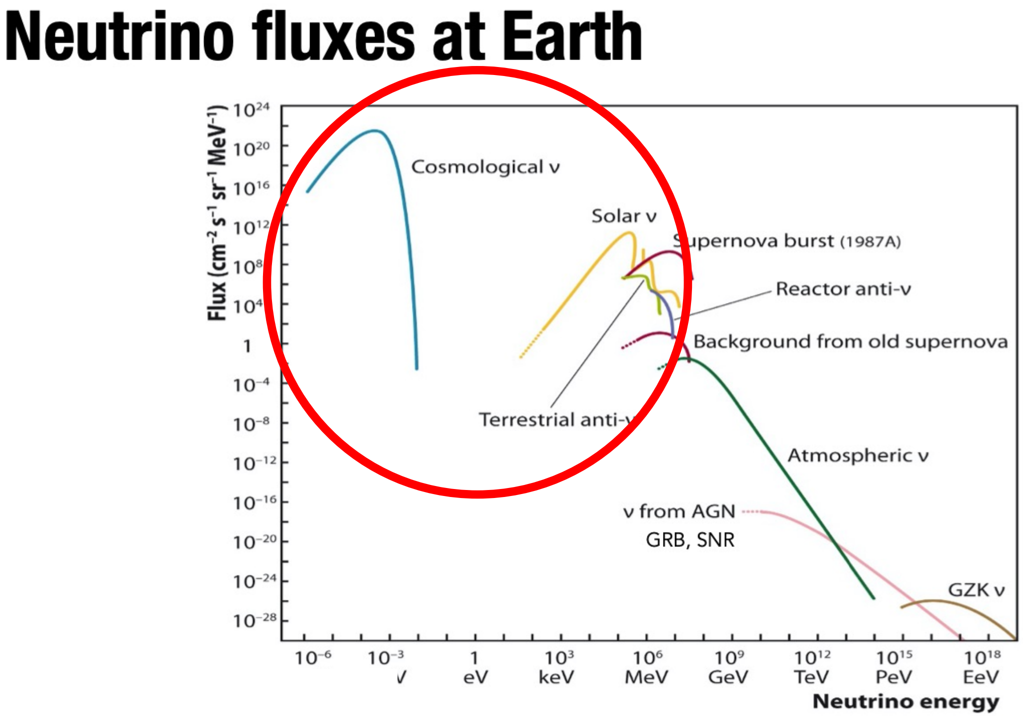
Other today's applications

Oscillations of neutrinos emitted
from Stellar objects

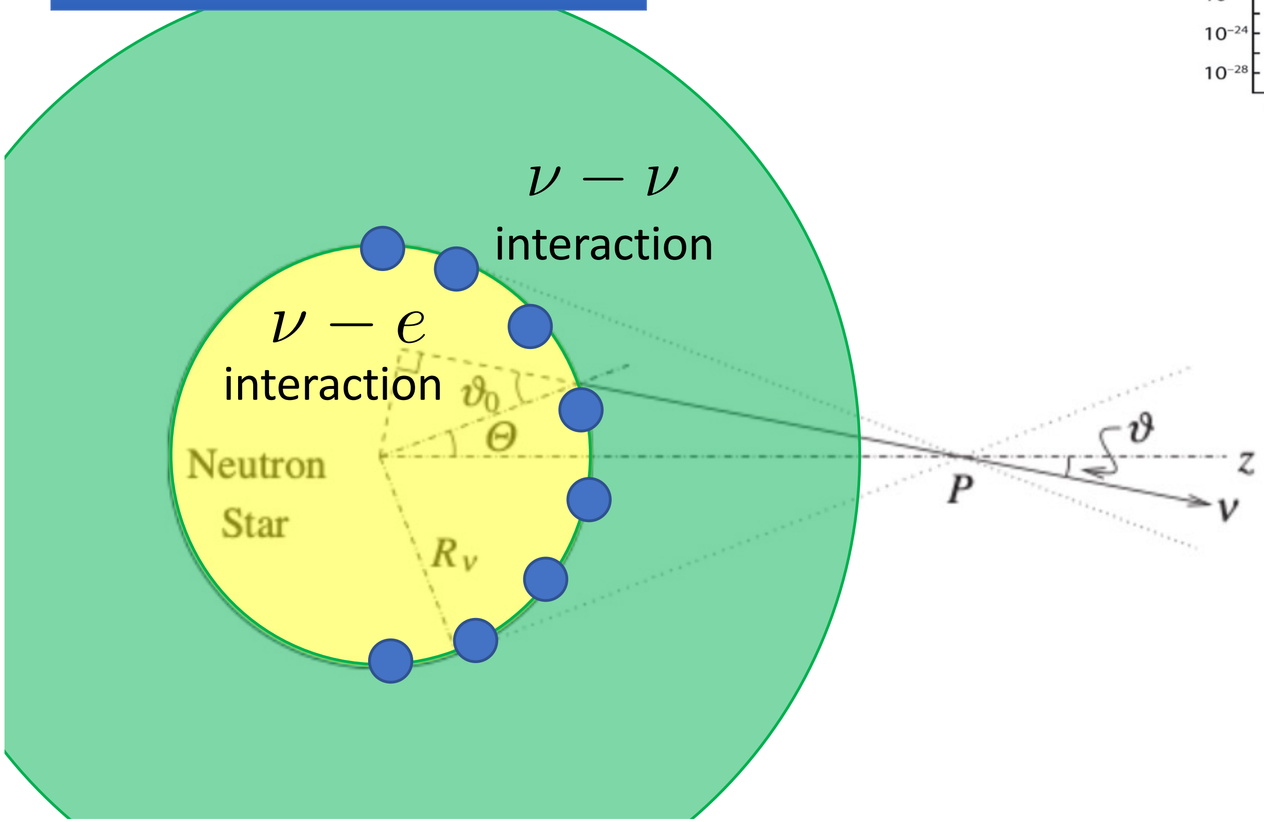








Where is the complexity?



The problem is mapped to a many-body open quantum system problem equivalent to interacting qubits or qutrits.

A focus on neutrino oscillation physics simulated on quantum computers

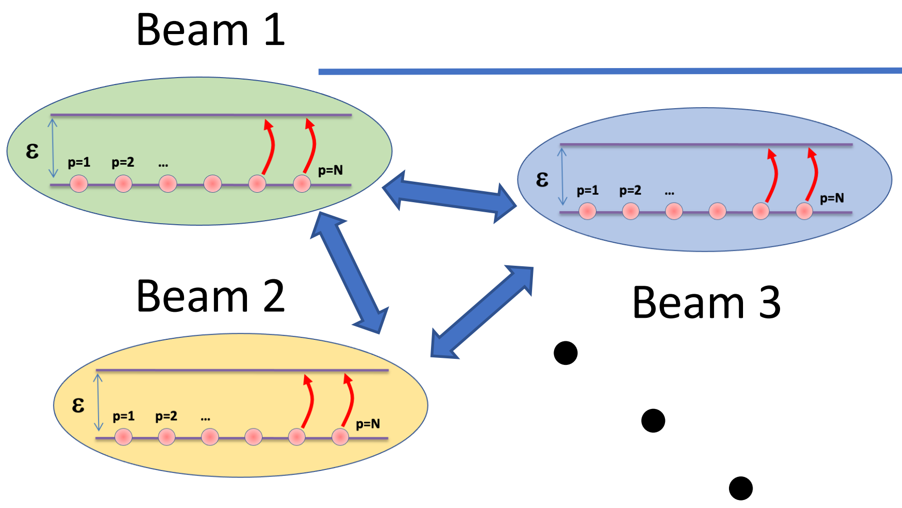


Illustration of the Hamiltonian (2 flavor approx)

Oscillation
$$H_\nu = \frac{1}{N}\sum_{i=0}^{N-1} \sin(2\theta_\nu)X_i - \cos(2\theta_\nu)Z_i$$

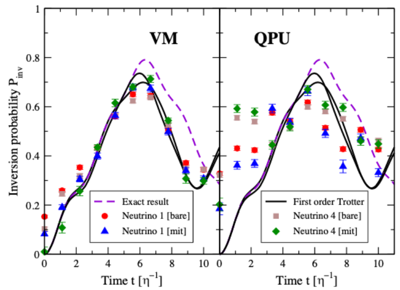
Coupling
$$H_{\nu\nu} = \sum_{i<j}^{N-1} G_{i,j}[X_iX_j + Y_iY_j + Z_iZ_j].$$

4 neutrinos
IBM-Vigo QPU

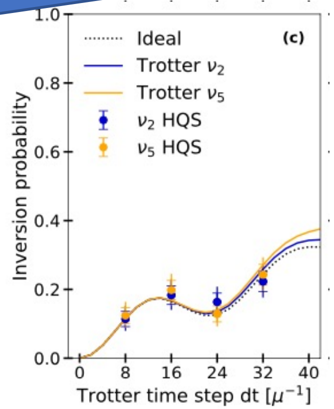
4 & 8 neutrinos
HQD-H1
Trapped Ion device

12 neutrinos
Quantinuum's H1-1
20 qubit trapped-ion

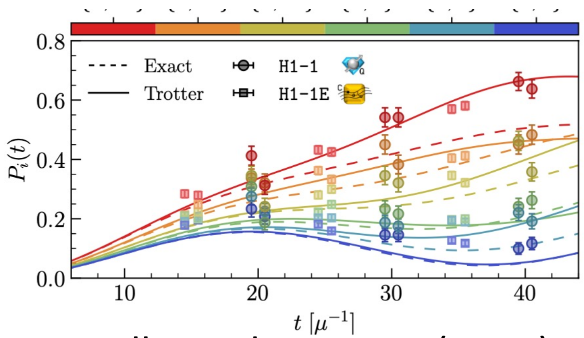
12 neutrinos / qutrits
H1-1 & ibm_torino



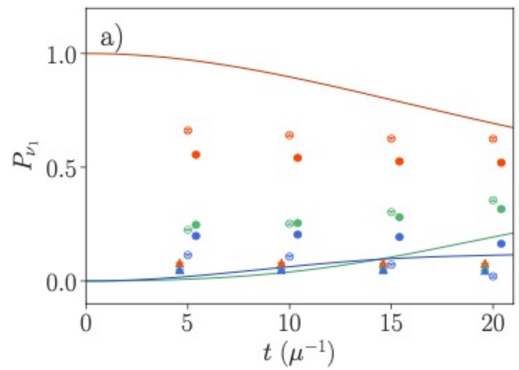
Hall et al, PRD 104 (2021)



Amitrano,et al, PRD 107, (2023)



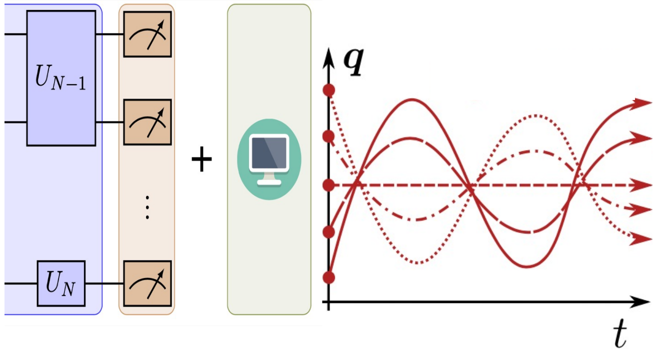
Illa et al, PRL 130 (2023)



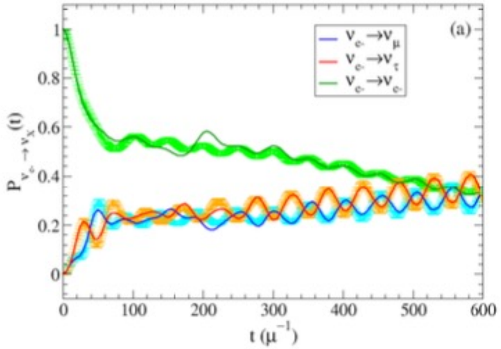
Turro et al,
PRD D 111 (2025)

Example 2: Neutrino oscillation physics

Two directions: - Simulation of neutrinos on qubits and qutrits
- Classical simulation on large qubits sets

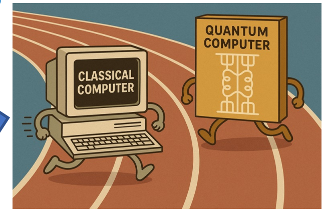


Lacroix et al, Phys Rev. D106 (2022), Phys Rev D110 (2024)



Mangin Brinet, Lacroix, PRD 13 (2026)

>100 neutrinos
IBM machines

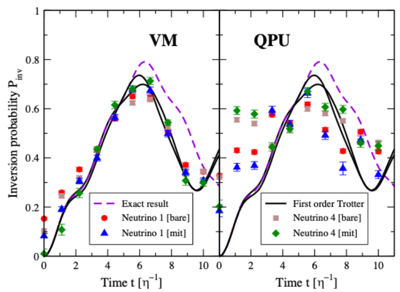


12 neutrinos / qutrits
H1-1 & ibm_torino

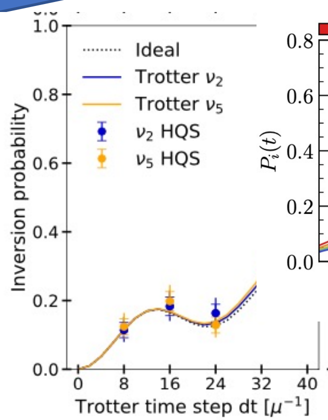
12 neutrinos
Quantinuum's H1-1
20 qubit trapped-ion

4 & 8 neutrinos
HQD-H1
Trapped Ion device
4 & 8 qubits

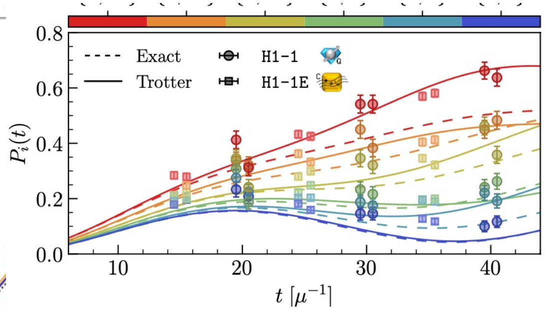
4 neutrinos
IBM-Vigo QPU
4 qubits



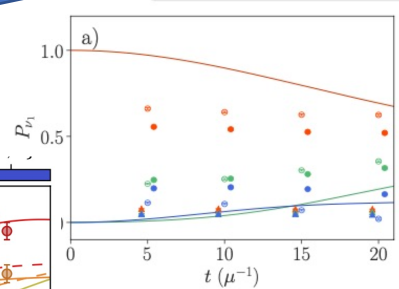
Hall, PRD 104 (2021)



Amitrano, PRD 107 (2023)

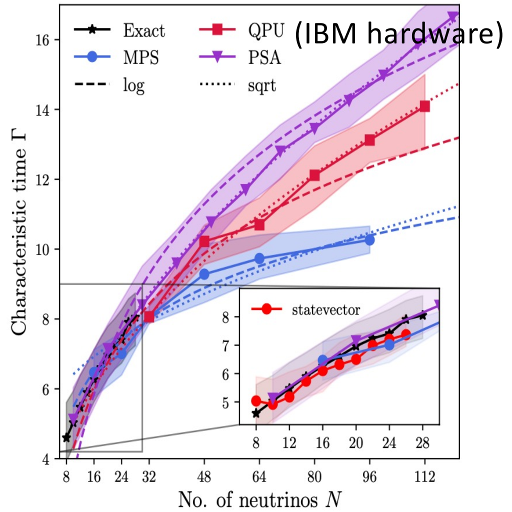


Illa, PRL 130 (2023)



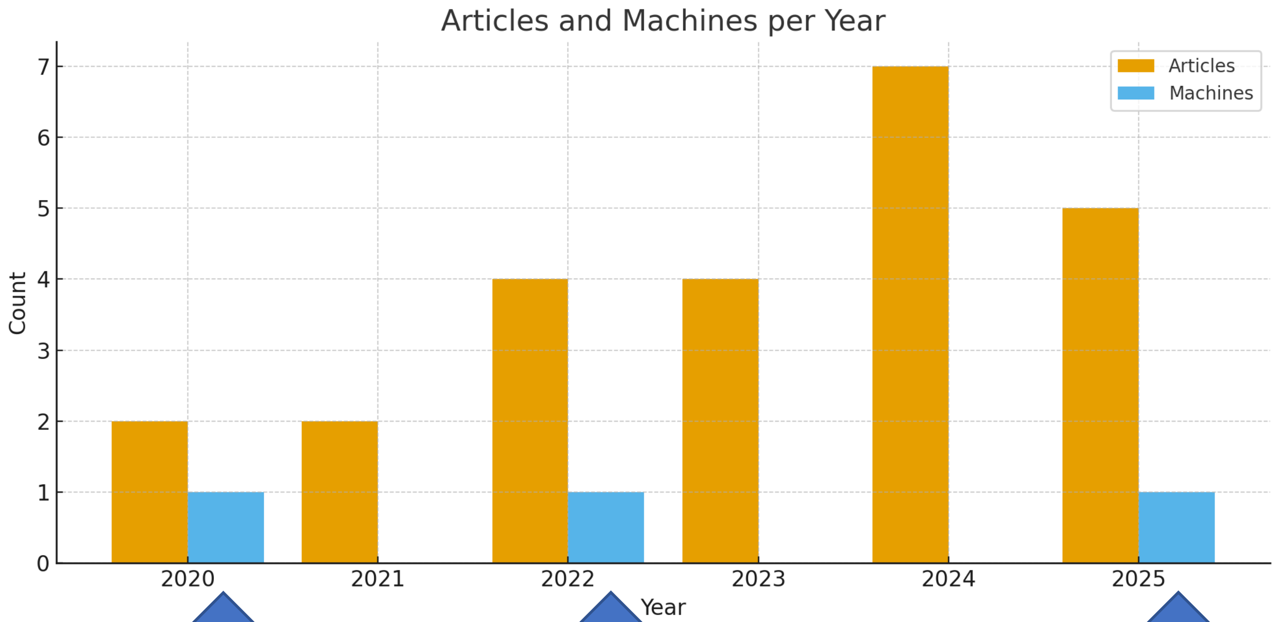
Turro, PRD 111 (2025)

Neutrino thermalization time

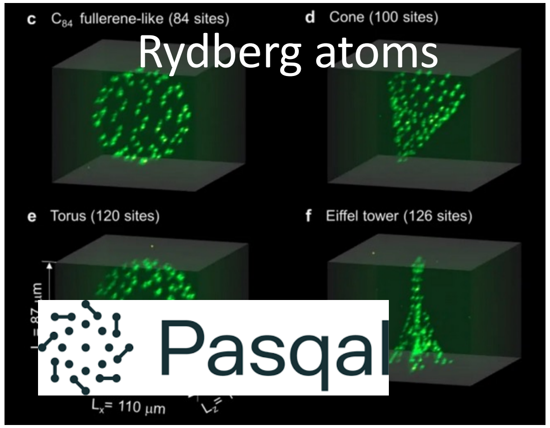


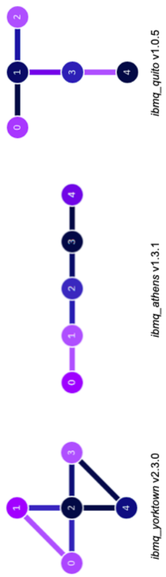
Kiss, Tavernelli, Tacchino, Lacroix, Roggero, arxiv:2510.24841

Real Quantum Machine access



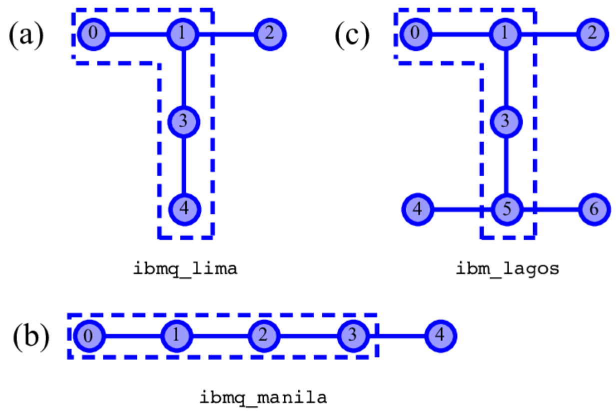
FRANCE HYBRID HPCQUANTUM INITIATIVE



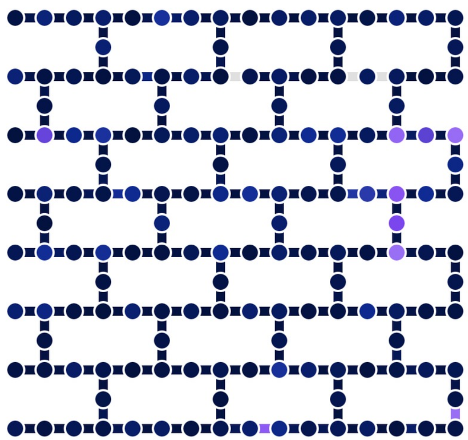


IBM Q5
(5 qubits)

IBM santiago,
manila, and bogota



ibm fez,
ibm aachen
(156 qubits)



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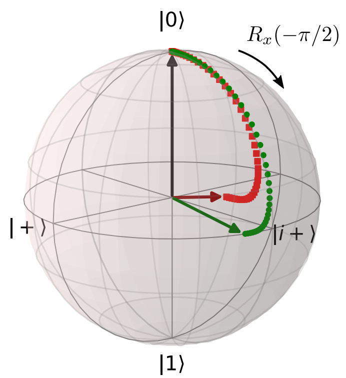
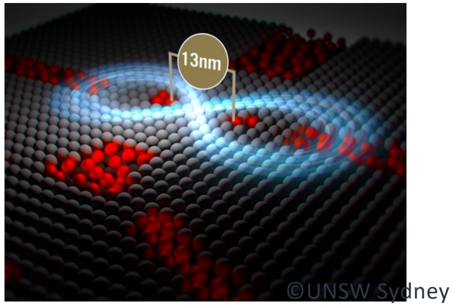
Thank you !

More on noisy devices
(if times allows)

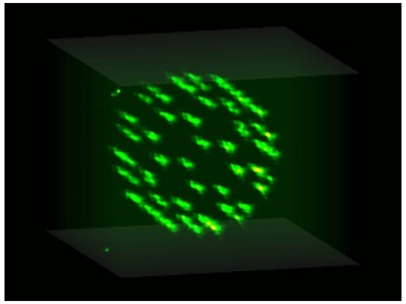
Quantum Hardware with noise
Noise description and
Noise mitigation



Many technologies are explored

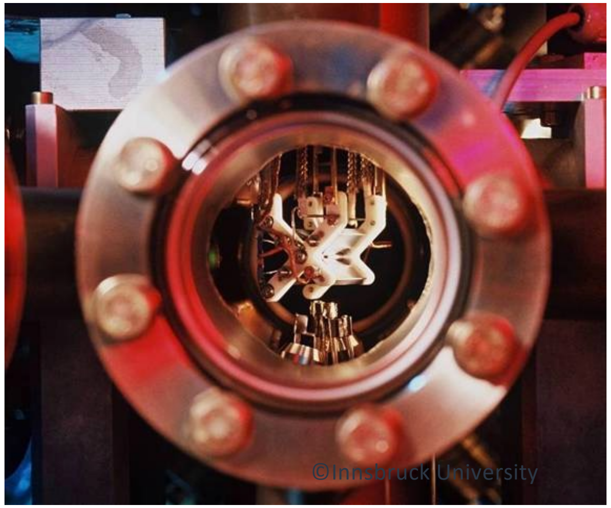


Silicon qubits

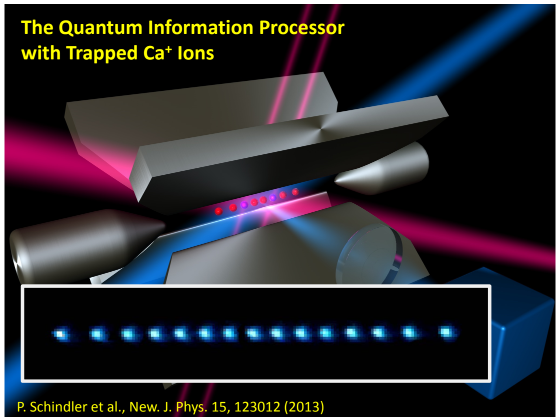


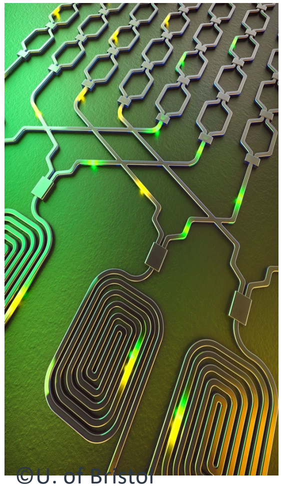
Neutral atoms

NMR

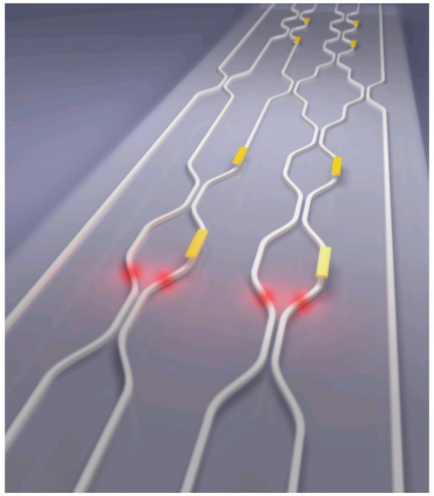


Trapped ions





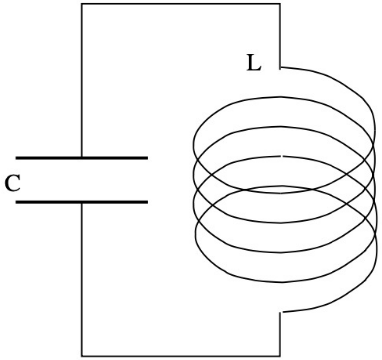
Photons



Superconducting qubits

Example 1: Superconducting qubits

Simple oscillator by LC circuit



$$H = \frac{1}{2L}\phi^2 + \frac{1}{2C}n^2$$

ϕ: flux in the inductor
n : charge in the capacitor

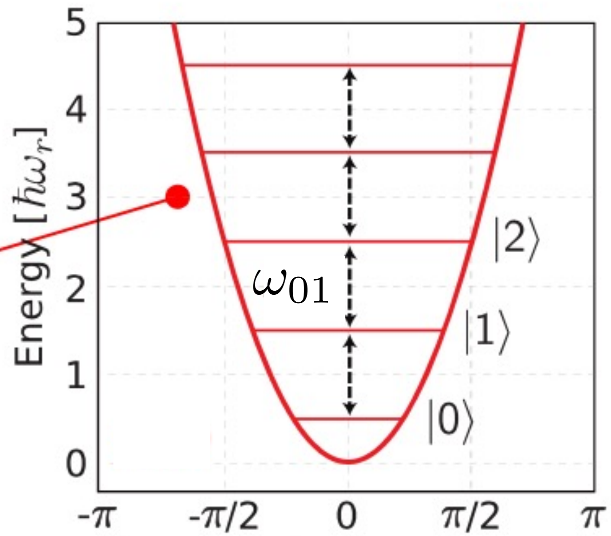
Methodology

- We consider the limit where quantum effects are important

$$k_B T \ll \hbar\omega_{01}$$

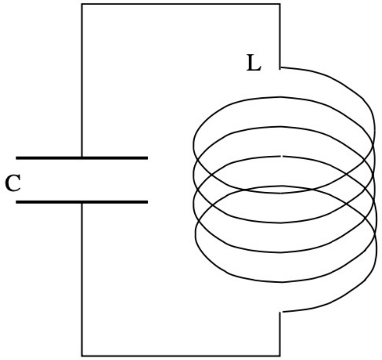
- n, ϕ becomes equivalent to canonical conjugated variables like *(x,p)* for the harmonic oscillator (HO)

Quantum HO



Example : Superconducting qubits

Simple oscillator by LC circuit

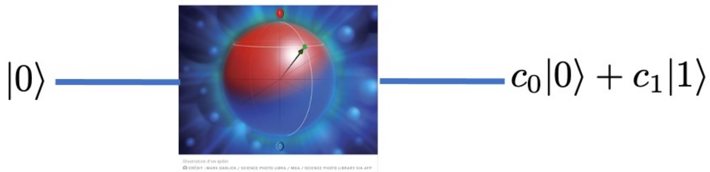


$$H = \frac{1}{2L}\phi^2 + \frac{1}{2C}n^2$$

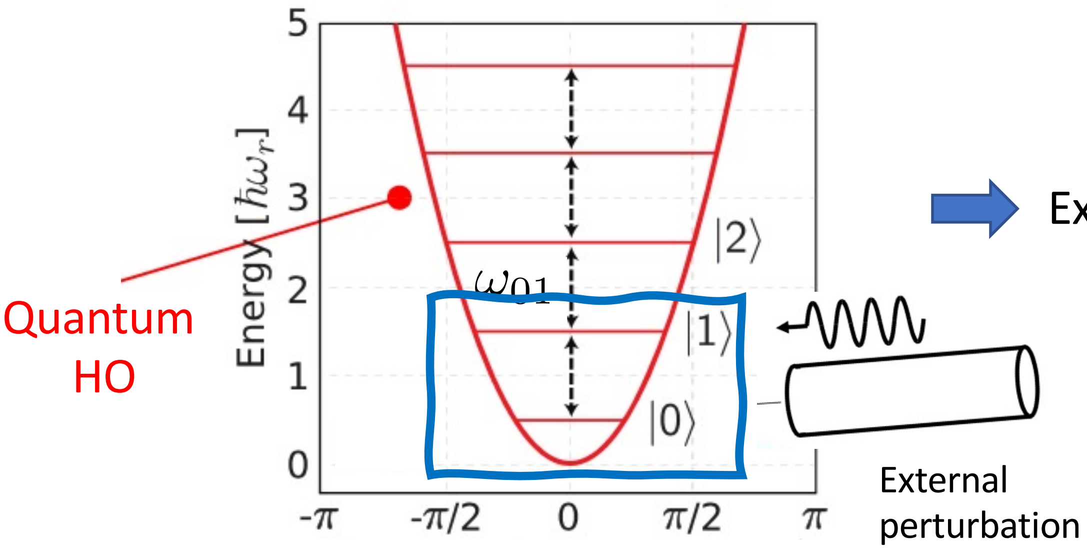
ϕ: flux in the inductor
n : charge in the capacitor

➡ We are interested in isolating $|0\rangle$ and $|1\rangle$

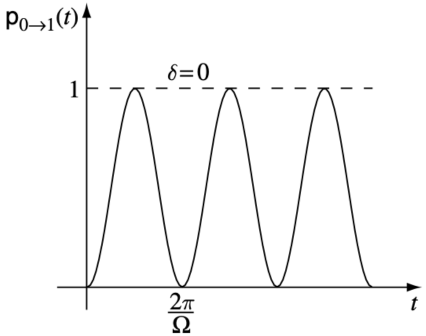
➡ We should prepare the system in any combination of them



Qubit identification and manipulation



➡ Example: induce Rabi-like oscillation



Two difficulties

Approximate operations

$$|0\rangle \longrightarrow |1\rangle$$

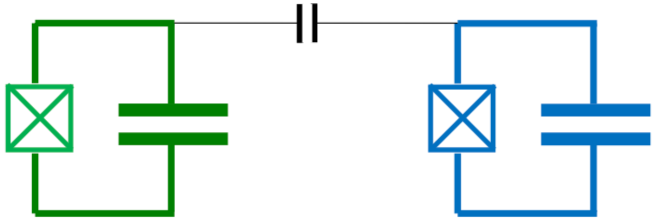
Unwanted transitions

$$|1\rangle \longrightarrow |2\rangle$$

Example: Superconducting qubits

Next step: putting several qubits together

2 qubits can be coupled through electrostatic interactions



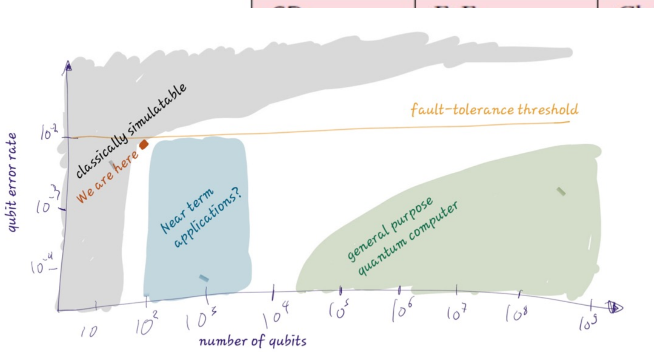
With this one can manipulate/entangle qubits

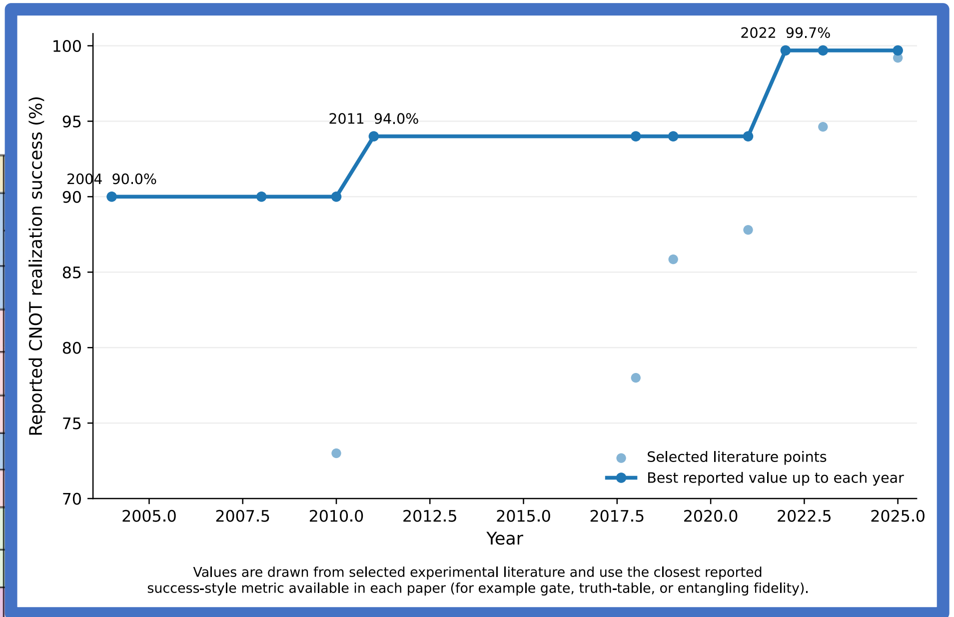
IBM Google rigetti IQM

Some specific Operations (see next lecture)

When

Acronym[b]	Layout[c]	First demonstration [Year]		
CZ (ad.)	T–T	DiCarlo et al. (72) [2009]		
√iSWAP	T–T	Neeley et al. (81)[d] [2010]		
[illegible]	[illegible]	...ow et al. (75)[h] [2011]		
[illegible]	[illegible]	...etto et al. (76) [2012]		
[illegible]	[illegible]	...ow et al. (77) [2013]		
[illegible]	[illegible]	...n et al. (55) [2014]		
[illegible]	[illegible]	...x et al. (78) [2016]		
[illegible]	[illegible]	...Kay et al. (79) [2016]		
[illegible]	[illegible]	...dwell et al. (80) [2018]		
[illegible]	[illegible]	...enblum et al. (13) [2018]		
[illegible]	[illegible]	...ou et al. (82) [2018]	79%[g] Chou et al. (82) [2018]	4.6 µs



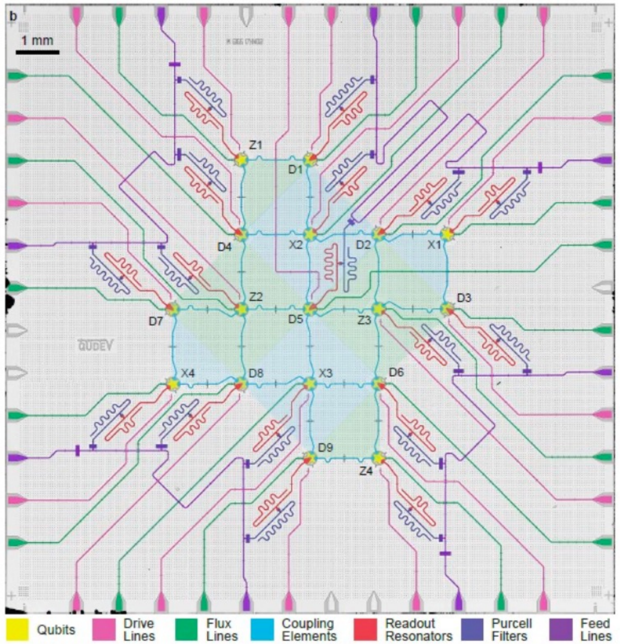


M. Kjaergaard, Annual Review of Cond. Matt (2020)

Where we are now ?

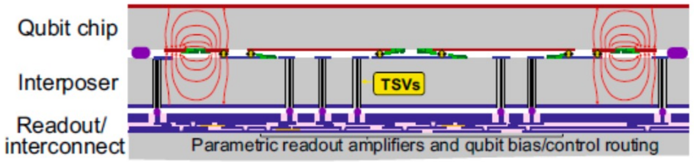
Example: Superconducting qubits

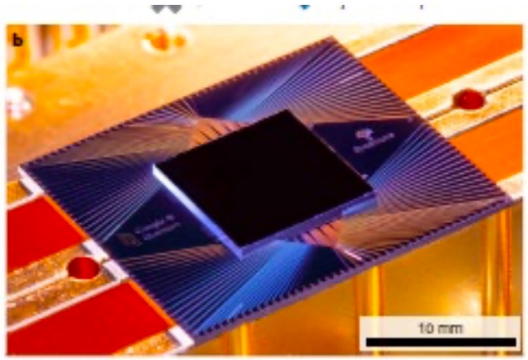
2D chip : 17 qubits



S. Krinner et al., arxiv (2021)
Wallraff group, ETHZ

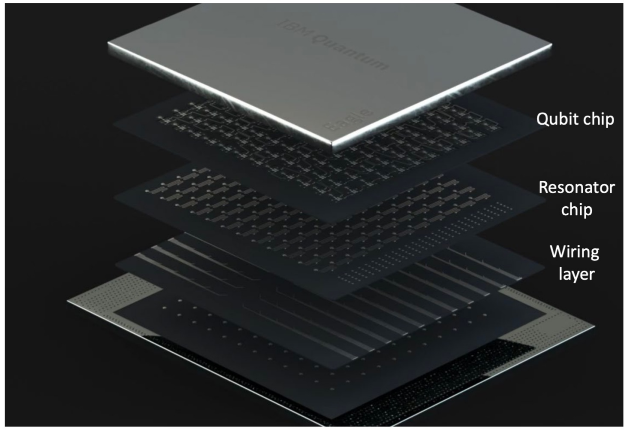
3D integration ~100 qubits demonstrated



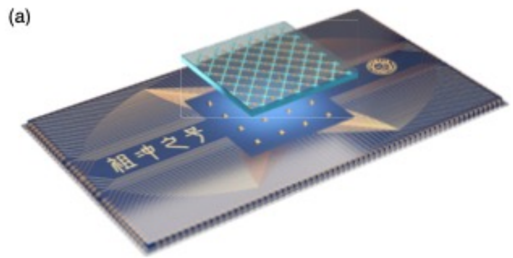


Rosenberg et al., NPJ (2017)
Arute et al., Nature (2019)

IBM Eagle
127 qubits



Zuchongzhi (66 qubits)
(PRL October 2021)



…

NISQ (Noisy intermediate Scale Quantum) period

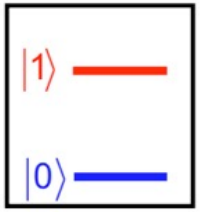
Many things tends to destroy the ideal qubits picture and the quantum coherence.

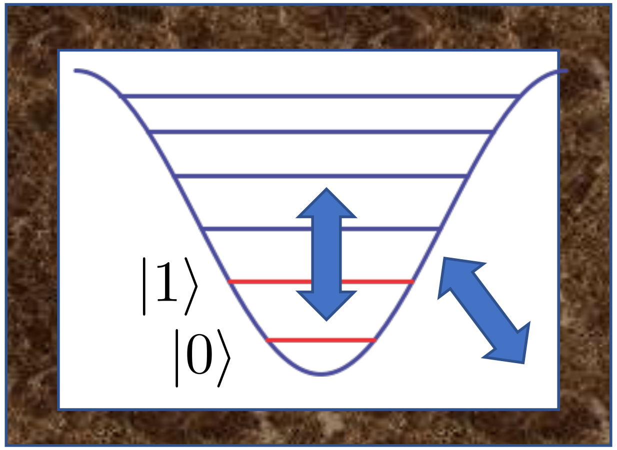
Leads to loss of information
And decoherence

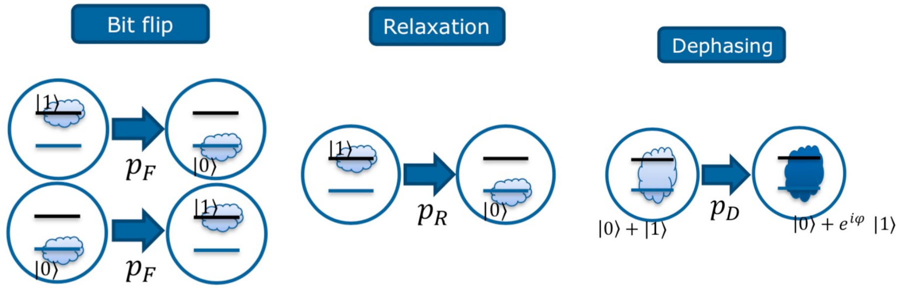
External Exp. Setup

Ideal Qubits

2 level system



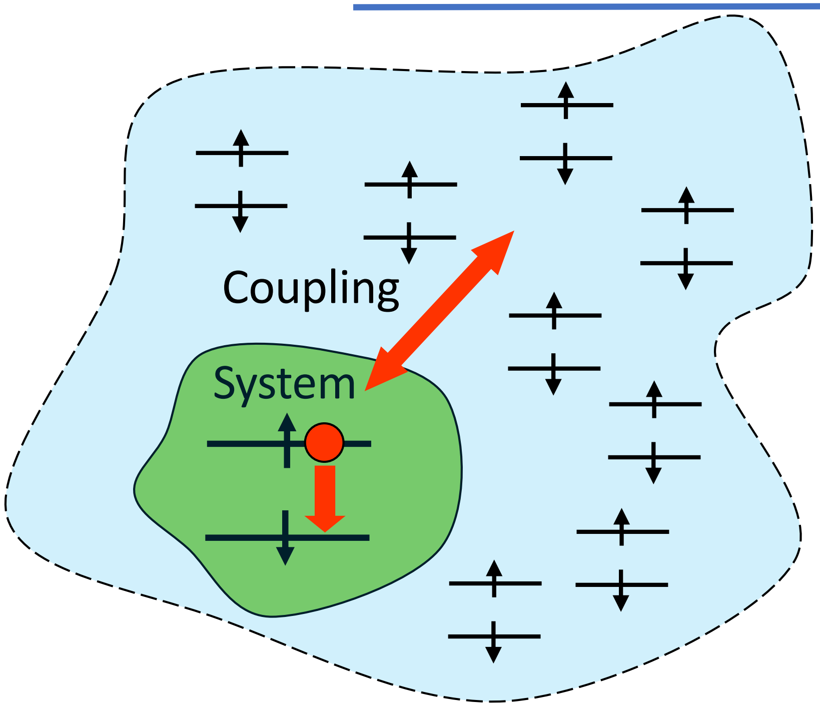




For multi-qubits, also cross-talk
(making operations on one qubit
Impacts other qubits)

NISQ period: Working with quantum computers now means working in a noisy environment and "NISQ friendly" programs, i.e. only selected algorithm can be applied and error mitigation should be made to get reasonable results.

Minimal notions on open quantum systems



Approximate system evolution

$$D(t) \xrightarrow{\text{Reduced system evolution}} \rho(t) = \mathrm{Tr}_{\mathrm{Env}} D(t)$$

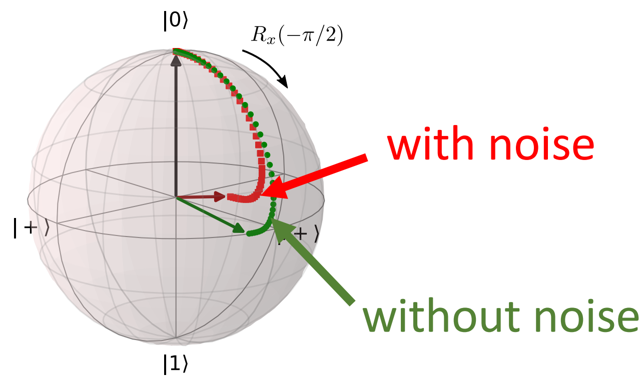
Assumptions:
-Weak coupling
-Env. More complex than system
-Markovian limit

Lindblad equation

$$\partial_t \rho = -i[h,\rho] + \sum_i \left(L_i^\dagger \rho L_i - \frac{1}{2} L_i^\dagger L_i \rho - \frac{1}{2} \rho L_i^\dagger L_i \right)$$

Gardiner and Zoller, Quantum noise (2000)
Breuer and Petruccione, The Theory of OQS, (2004)

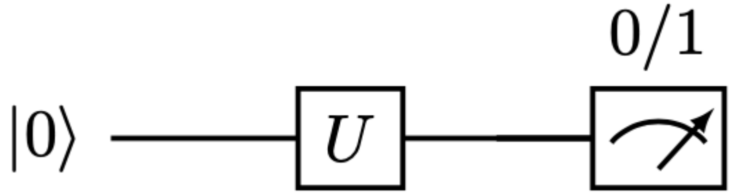
- Dephasing $L_i = \sqrt{\gamma_i} Z_i$
- Amplitude damping $L_i = \sqrt{\gamma_i} \sigma_i^-, \quad \sqrt{\gamma_i} \sigma_i^+$
- Depolarization $L_i = \sqrt{\gamma_i} X, \quad L_i = \sqrt{\gamma_i} Y, \quad L_i = \sqrt{\gamma_i} Z$



How to correct from the imperfect quantum computers

Readout error mitigation

Circuit efficiency



Perform many events to get the probability to mesure one and zero for specific states

Prepared state	Ideal meas.		Reality	
	0	1	0	1
$\|0\rangle$	1	0	0.96	0.04
$\|1\rangle$	0	1	0.18	0.82

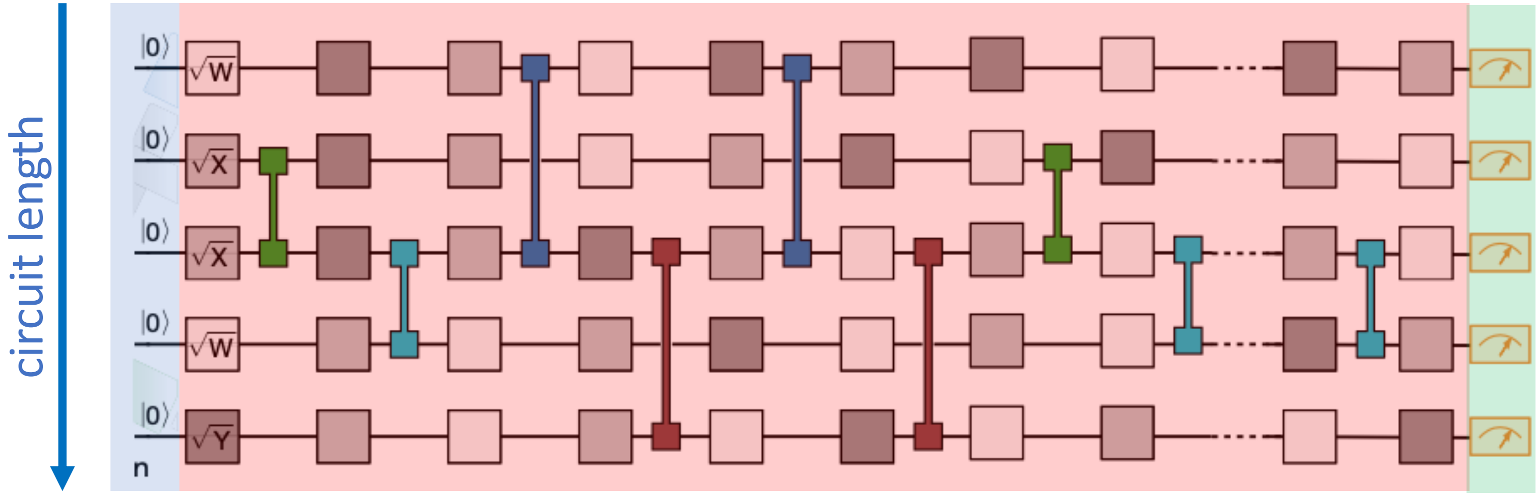
$$\begin{pmatrix} p_0 \\ p_1 \end{pmatrix}_{\text{noisy}} = \begin{pmatrix} 0.96 & 0.04 \\ 0.18 & 0.82 \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \end{pmatrix} \equiv M \begin{pmatrix} p_0 \\ p_1 \end{pmatrix}$$

$$\begin{pmatrix} p_0 \\ p_1 \end{pmatrix} = M^{-1} \begin{pmatrix} p_0 \\ p_1 \end{pmatrix}_{\text{noisy}}$$

One difficulty is that the dimension of M scales exponentially with the number of qubits

How to correct from the imperfect quantum computers

Purification techniques



Test specific properties

$$01 \cdots 001$$

Example of fermions

- -Number of particles
- -N-representability
- -Testing the purity of states

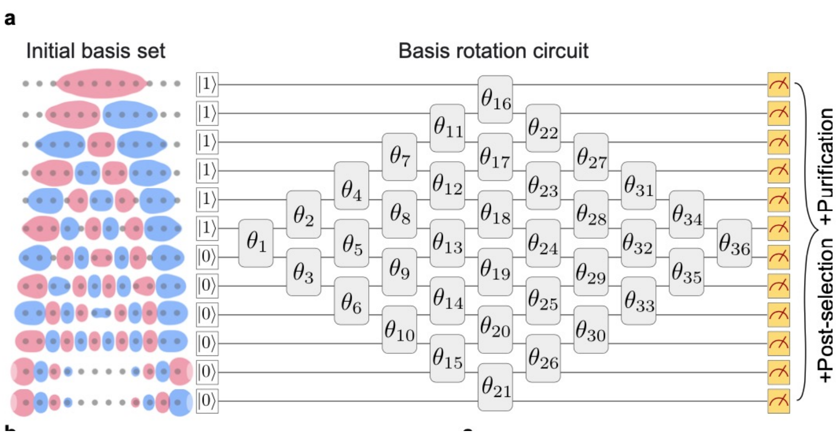
$$\rho^2 - \rho = 0$$

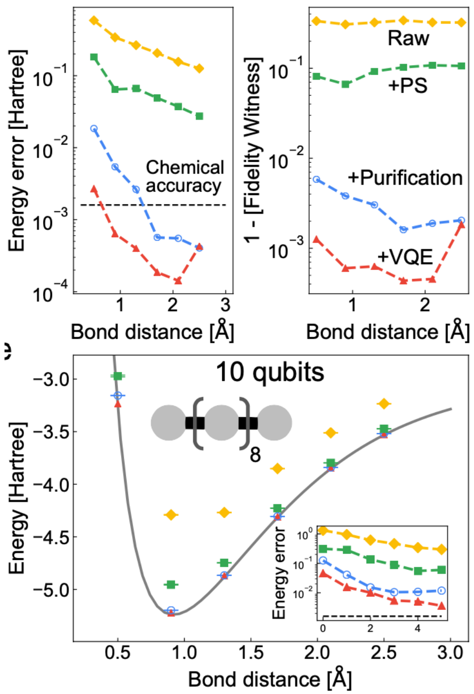
$$\cdots$$

Example 1-RDM purification

Hartree-Fock on a superconducting qubit quantum computer

Google AI Quantum and Collaborators*
(Dated: September 22, 2020)





How to correct from the imperfect quantum computers

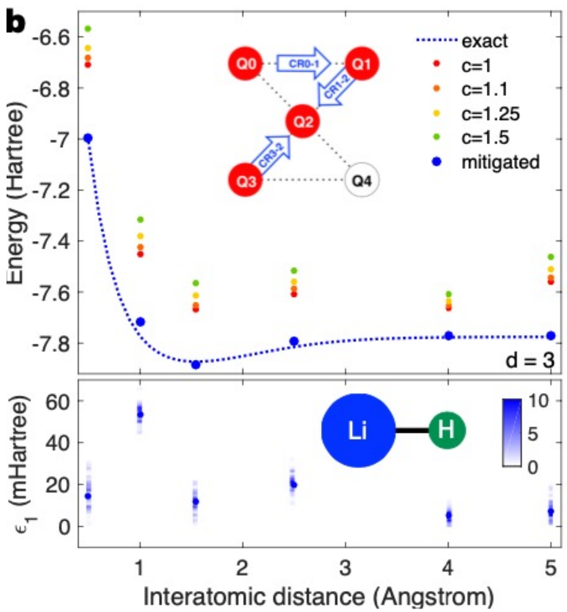
Zero noise interpolation

$$\partial_t \rho = -i[h,\rho] + \boxed{\gamma} \sum_i \left(L_i^\dagger \rho L_i - \frac{1}{2} L_i^\dagger L_i \rho - \frac{1}{2} \rho L_i^\dagger L_i \right)$$

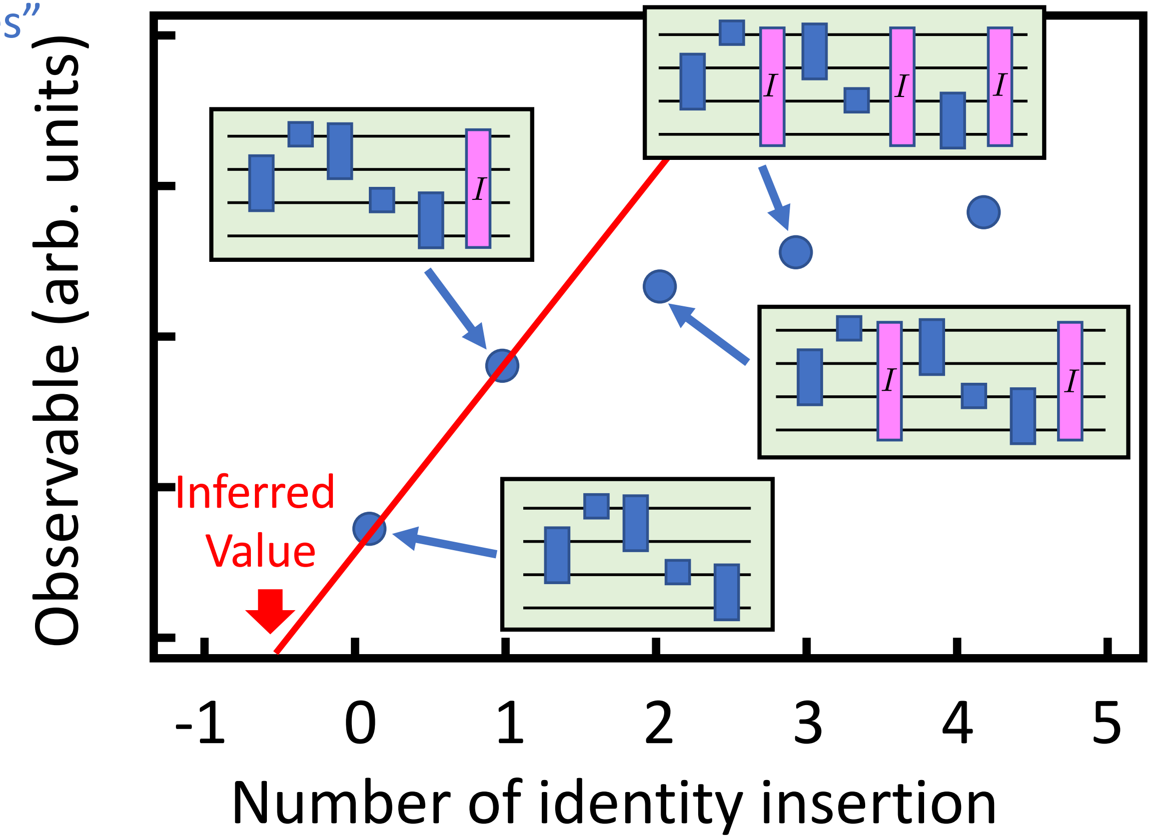
Assumes that noise scales linearly with the circuit length (number of gates)

Zero Noise extrapolation (ZNE)

The main idea: add artificially “useless gates”
And make linear interpolation



Kandala et al, Nature 567, 491 (2019)



How to correct from the imperfect quantum computers

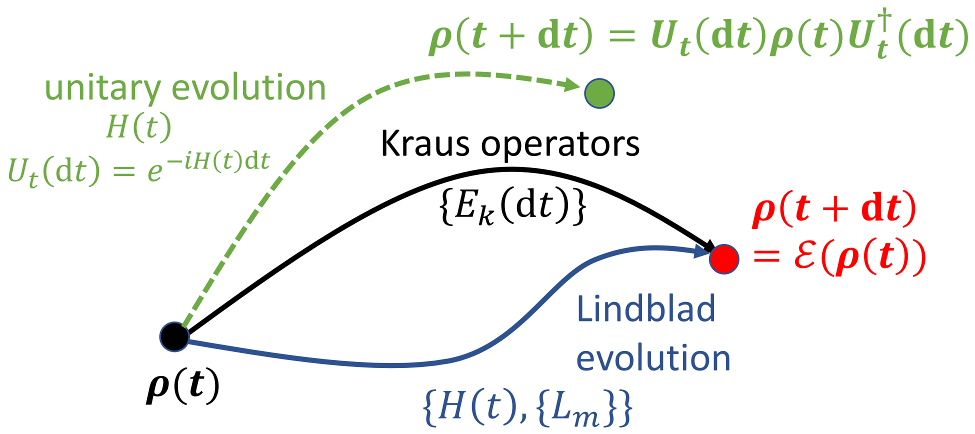
Probabilistic corrections to the noise

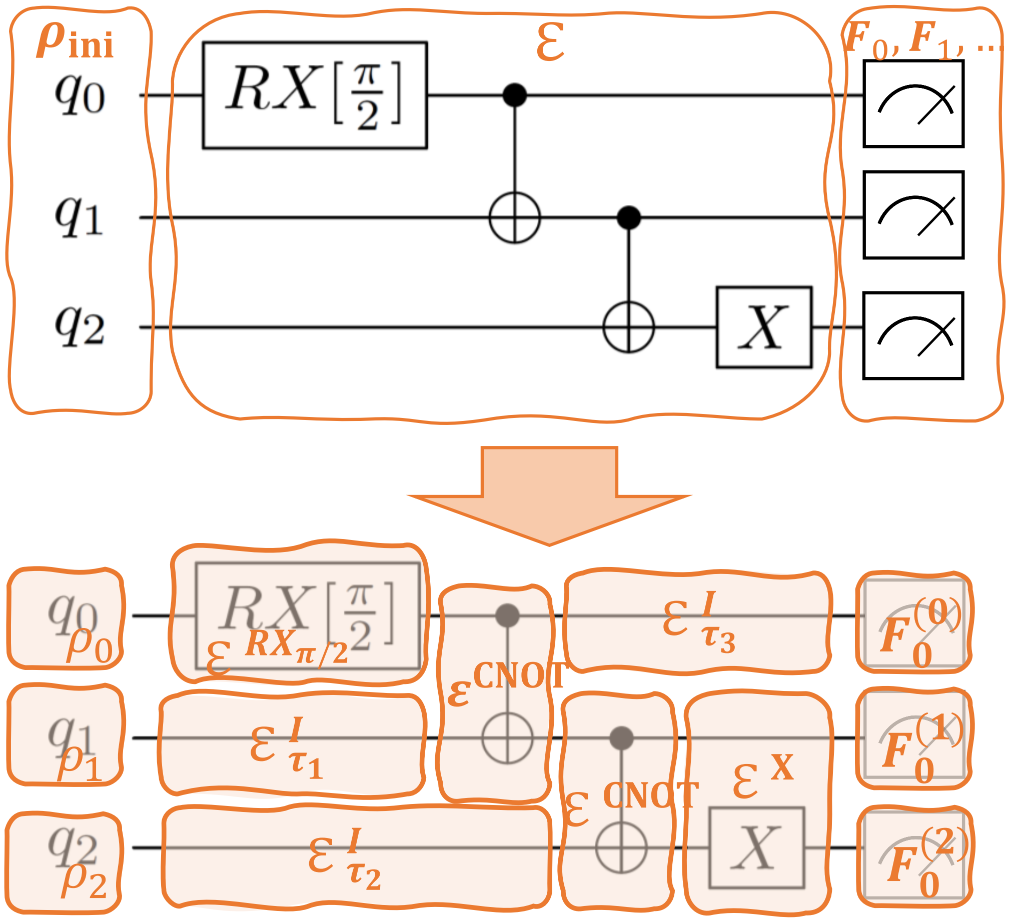
Kraus operator

Kraus operators connect noisy and noiseless channels

$$\mathcal{E}(\rho) = \sum_{k=1}^{K} E_k \rho E_k^\dagger$$

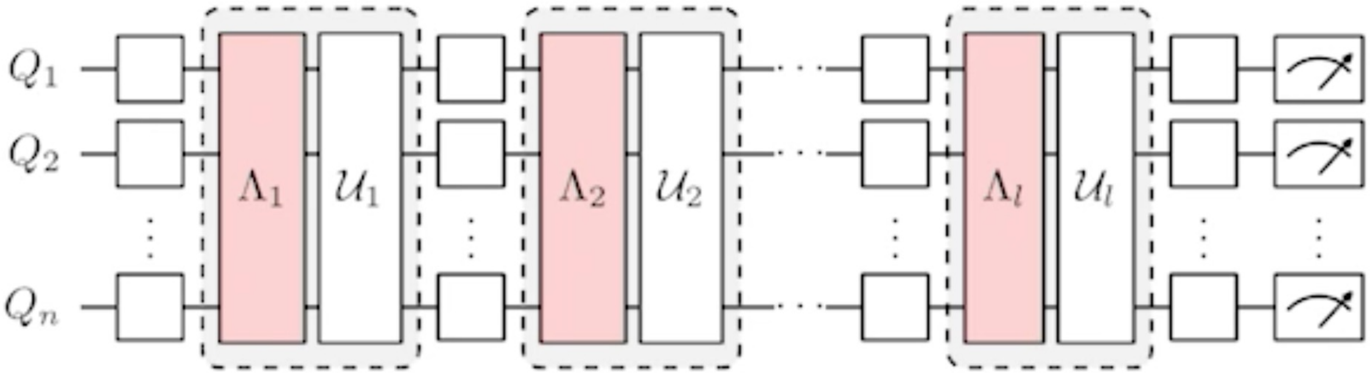
The Kraus operator decomposition can be seen as an alternative to Lindblad





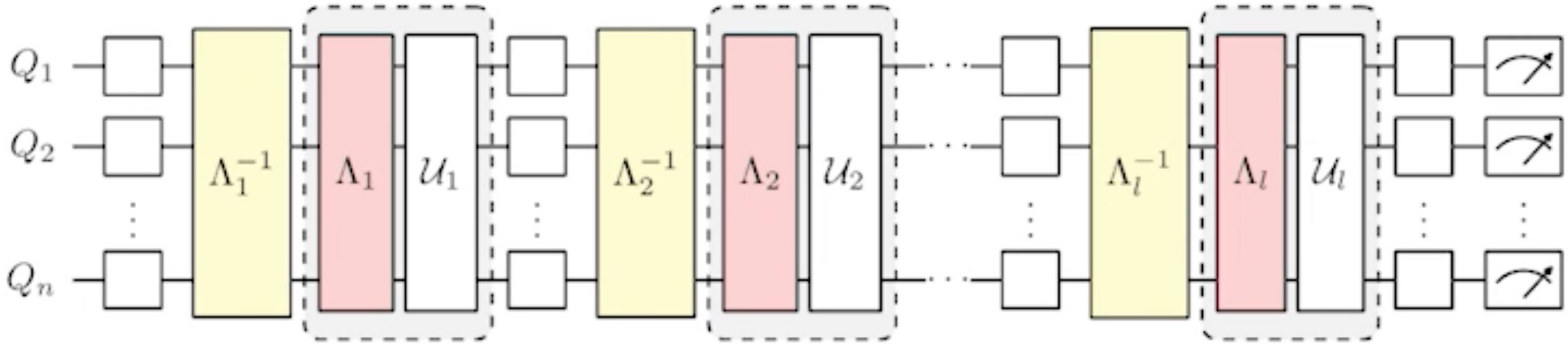
(see Ayral et al, EPJA 59 (2023))

Imagine the noise is perfectly known (i.e. it is associated to a set of operations)



$\{\Lambda_i\}$ =Noise channels operations

Ideally we would like to compensate for the noise



Problem Usually noise channels cannot be described by physical/unitary operations
The dimension of matrices growth exponentially.

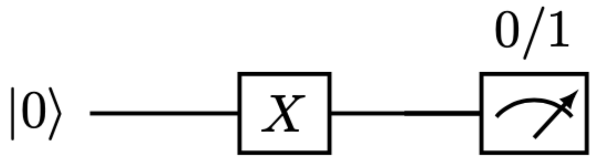
https://open.hpi.de/courses/qc-nature2023/

How to correct from the imperfect quantum computers

Probabilistic corrections to the noise

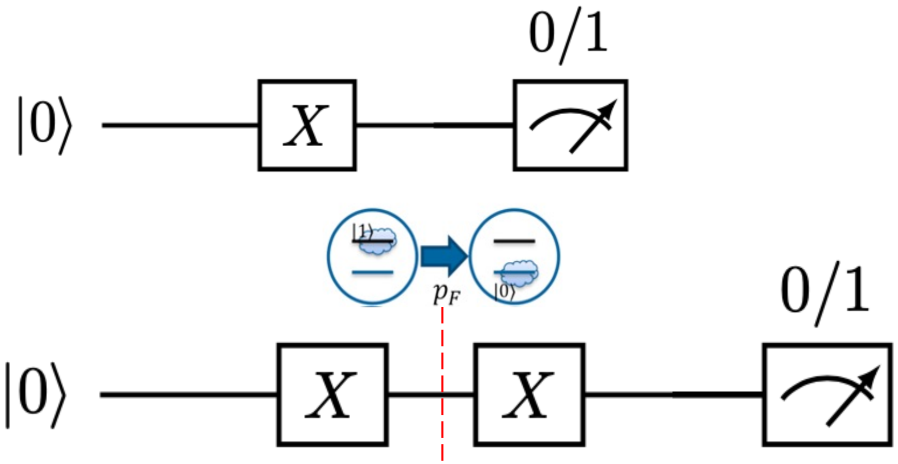
The idea is to correct it statistically

Sampling circuit technique



Should gives always 1 but gives 1 with probability p_1

The idea is that spin flip can be corrected by adding sometimes an extra gate X or not



Random circuit will be added statistically

Temme et al, PRL 119 (2017)

(and many more techniques …)

Quantum error mitigation: (Non-exhaustive) literature

Zero Noise Extrapolation

Key feature: Noise scaling

K. Temme, et al., **Phys. Rev. Lett.** (2017)
A. Kandala, et al., **Nature**, 567, 491 (2019)
T. Giurgica-Tiron et al., **IEEE Trans.Q.Comp** (2021)
I. Chen, et al., arXiv:2203.08291
E. Huffman *et al.* arxiv:2109.15065

Probabilistic Error Cancellation & Quasi-Probabilistic Repr.ns

Noisy gate-level representation

K. Temme, et al., **Phys. Rev. Lett.** (2017)
H. Pashayan, et al., **Phys. Rev. Lett.** 115, 070501 (2015)
S. Zhang, et al., **Nature Commun.** 11, 587 (2020)
A. Mari et al.,. **Phys. Rev. A** 104, 052607 (2021)
R. LaRose, et al., arXiv:2009.04417 **Quantum** (2022)
C. Piveteau, *et al.*, **Phys Rev Lett.** 127 200505 (2021)
E. van den Berg, arXiv:2201.09866

Learning-based Methods

Learn noise (ML), use Clifford circuits

P. Czarnik et al., **Quantum** 5, 592, (2021)
A. Strikis, et al., **PRX Quantum** 2, 0(2021)
A. Lowe et al., **Phys. Rev. Res.** 3, 033098 (2021)
Z. Cai, **NPJ Qu. Inf.** 7, 1 (2021)

Symmetry-based Techniques

Key feature: Noisy state re-projected

J. R. McClean, et al., **Phys. Rev. A** 95, 042308 (2017)
X. Bonet-Monroig, et al., **Phys. Rev. A** 98, 062339 (2018)
J. R. McClean, et al., **Nature Commun.** (2020)
R. Sagastizabal, et al., **Phys. Rev. A** 100, 010302 (2019)

Dynamical Decoupling & Randomized Compiling

Add gates to protect from 'bad' noise

L. Viola et al., **Phys. Rev. A** 58, 2733 (1998)
L. Viola et al., **Phys. Rev. Lett.** 82, 2417 (1999)
J. Zhang, et al., **Phys. Rev. Lett.**112, 050502 (2014)
B. Pokharel et al., **Phys. Rev. Lett.** 121, 220502 (2018)
J. J. Wallman, J. Emerson, **Phys. Rev. A** 94, 052325 (2016)

Other research

Mix of / specific approaches

R. M. Parrish, et al. **Phys. Rev. Lett.** 122, 230401 (2019)
P. J. J. O'Malley, et al., **Phys. Rev. X** 6, 031007 (2016)
T. Proctor et al. **Nature Phys.** 18, 75 (2021)
Y. Li, S.C. Benjamin **Phys. Rev. X** 7, 021050 (2017)
Jinzhao Sun, et al, **Phys. Rev. Appl.** 15, 034026 (2021)
R. Takagi, **Phys. Rev. Res** (2021)
E. Knill. **Nature** 434, 39 (2005)
S. Endo et al. **Phys. Rev. X** 8, 031027 (2018)
Loock, **Phys. Rev. A** 89, 022316 (2014)

Review: S. Endo, *et al.*, Hybrid quantum-classical algorithms and quantum error mitigation. J. Phys. Soc. Japan, 90, 032001 (2021) arXiv:2011.01382

See also the recent review: Cai et al, Rev. Mod. Phys. 95 (2023))

All references at:

https://mitiq.readthedocs.io/en/stable/

(slide from Nathan Shammah talk - SQMS Summer School, 26th July 2022 Galileo Galilei Institute, Florence, Italy)

Some challenges to face when working with larger number of qubits

Working with more and more qubits allows to work with exponentially growing matrix sizes

This also might lead to an exponential number of operations to do

This also lead to an exponentially growing number of measurements to be made. Leading to large data flow to treat classically

For instance full quantum tomography would require to estimate 4^n operators

Even a very small error for each gate will propagate exponentially with the number of operators

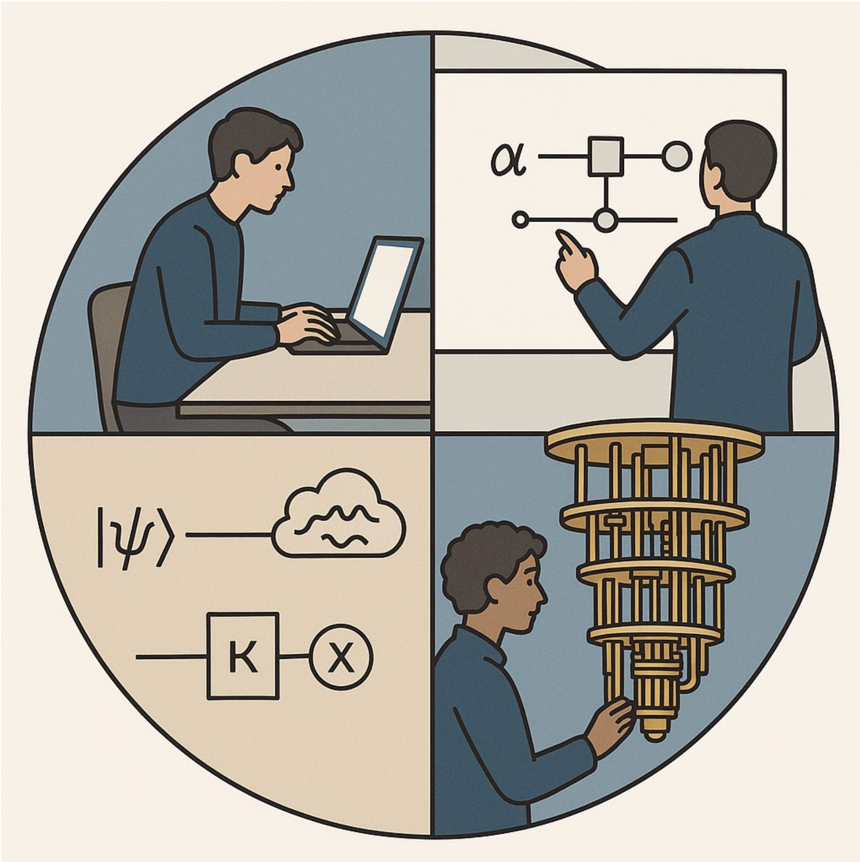
$$0.99^{\left(4^8\right)} \simeq 9.10^{-287}$$

High-level summary

The domain is at the Crossroad between physics, math, informatics

...

and experimental aspects
(signal processing, error corrections, real-time data analysis, crosstalk ...)



We are gaining expertise in quantum algorithms.

Applications are mainly on pilot applications

We now explore (ab-initio) non-equilibrium phenomena, entanglement properties, ...

Experimental platforms are improving fast worldwide. Access to them might rapidly be an issue

Special Thanks to

2020

E. A. Ruiz Guzman [PhD 2020-2023]

Quantum state preparation and many-body Methods on QC

2021

Y. Beaujeault-Taudiere [Postdoc 2021-2023]

Exploration of quantum machine learning technique for nuclear physics.

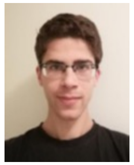
2022

2023

J. Zhang [PhD 2021-2025]

Neutron-Proton pairing on quantum computers

2024



S. Aychet Claisse [PhD 2023-2026]

Simulation of nuclear physics problems on quantum computer

2025

C. de Correc [PhD 2025-2028]

Annealing method for many-body methods

2026

R. Bocquet[PhD 2026-2029]

Quantum Computing for Nuclear Spectroscopy

A.Singh [Postdoc 2026-2028]

Ab-initio methods (Lattice EFT), resonances

Thanks to my Collaborators

Nuclear Physics

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Vittorio Somà

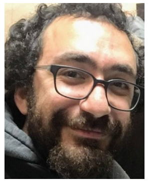
P. Siwach

Neutrinos Physics

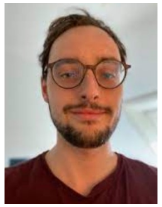
LPSC Grenoble, Laboratoire de Physique Subatomique et de Cosmologie — The University of Wisconsin Madison — Università di Trento — CERN — IBM Quantum

M. Mangin Brinet

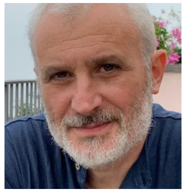
B. Balantekin



A. Roggero



O. Kiss



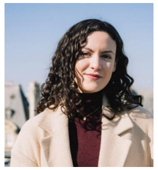
F. Tavernelli

F. Tacchino

General Quantum computing/many-body/Quantum Machine Learning

École Polytechnique IP Paris — QSL Quantum Software Lab — EVIDEN an atos business — Alice & Bob — ICGM Institut Charles Gerhardt Montpellier — Universidad de Sevilla 1505

T. Ayral



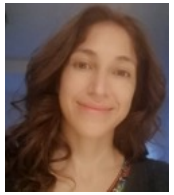
P. Besserve

C. Bertrand

F. Jamet

B. Senjean

Jesus pascual Casado



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