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Quantum Computing with Neutral Atoms

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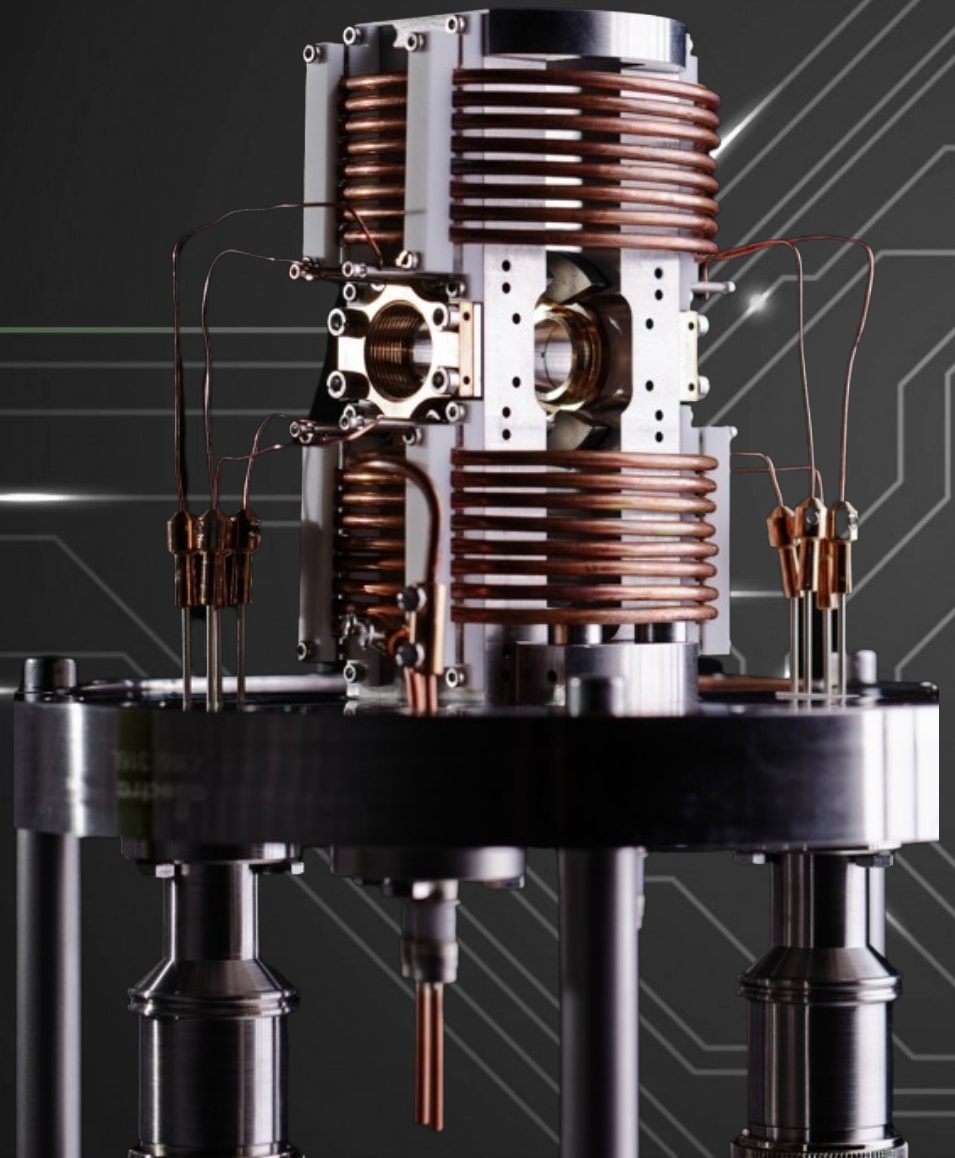


Recap of hydrogen atom

Infinitely massive proton sitting in the origin and generating a Coulomb potential

Schrodinger equation: $\left(-\frac{\nabla^2}{2}-\frac{1}{r}\right)\psi = W\psi$

- $\psi =$ electron wave function
- $W =$ electron energy
- $r =$ electron distance from proton

Assume the wave function is separable in radial and angular part: $\psi = Y(\theta,\phi)R(r)$

SE in spherical coordinates becomes:

$$\underbrace{\frac{r^2}{R}\left[\frac{\partial^2 R}{\partial r^2}+\frac{2}{r}\frac{\partial R}{\partial r}+2\left(W+\frac{1}{r}\right)R\right]}_{\text{Solution: Coulomb functions f and g}}+\underbrace{\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial Y}{\partial^2\phi}\right]}_{\text{Solution: spherical harmonics}}=0$$

Recap of hydrogen atom

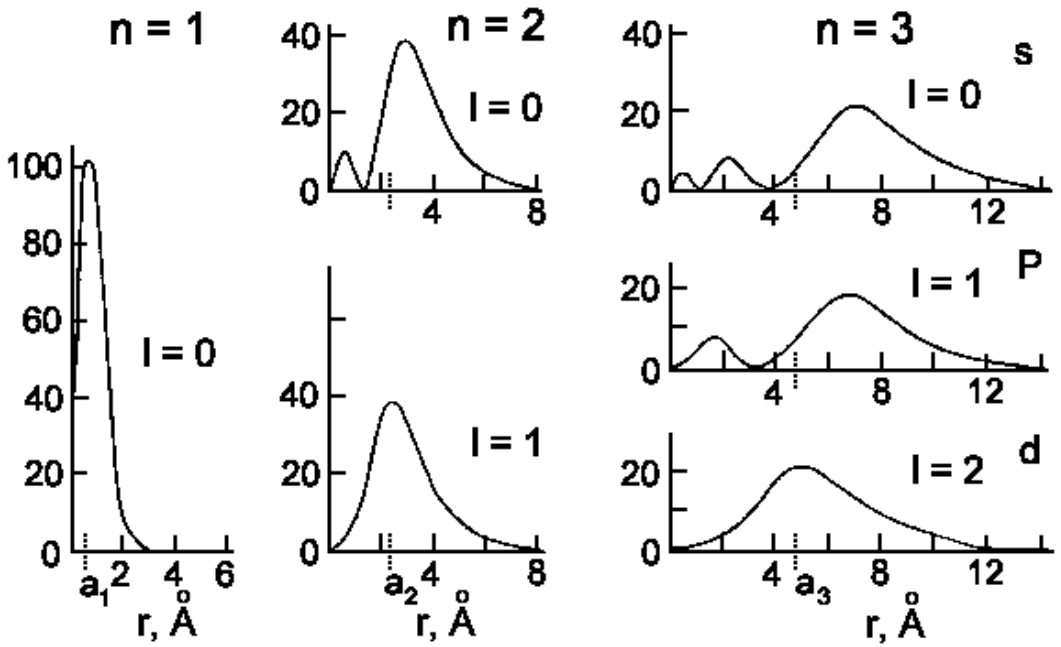
Electron wavefunction

$$\psi_{nlm}(\theta,\phi,r) = \frac{1}{r} Y_{lm}(\theta,\phi) f(W,l,r)$$

Allowed energies

$$W = -\frac{1}{2n^2}$$

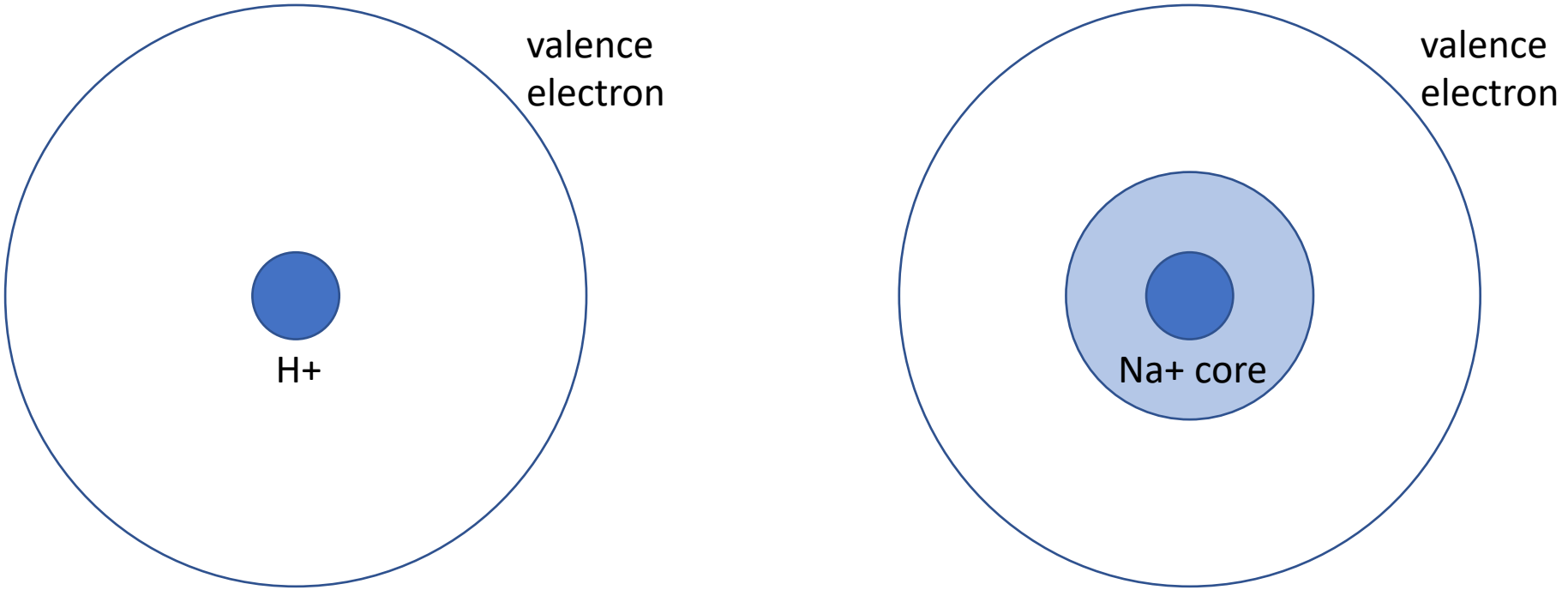
g function is excluded by boundary conditions



Radial probability distribution for various n and l

Alkali metals

The elements in the first column of the periodic table all have just one valence electron (Li, Na, K, Rb, Cs, Fr)



Alkali metals

The valence electron in an alkali metal feels the same Coulomb potential of a hydrogen atom for large r, but for small r the finite-size of the ionic core changes the potential

Large r

For large r, the potential felt by the valence electron is basically a Coulomb potential given by the net +1 charge of the inner core (N protons + (N-1) electrons)

Schrodinger equation: $\left(-\frac{\nabla^2}{2}-\frac{1}{r}\right)\psi = W\psi$

(same as hydrogen)

Small r

If r is less than the radius of the inner core, the valence electron feels a different potential

Schrodinger equation: $\left(-\frac{\nabla^2}{2}+V\right)\psi = W\psi$

with $V \neq -\frac{1}{r}$

Alkali metals

Consequence: for r large enough, there's an l-dependent correction denoted δ_l (defect)

Hydrogen

$$\psi_{nlm}(\theta,\phi,r) = \frac{1}{r}Y_{lm}(\theta,\phi)f(W,l,r)$$

$$W = -\frac{1}{2n^2}$$

Alkali metals

$$\psi_{nlm}(\theta,\phi,r) = \frac{1}{r}Y_{lm}(\theta,\phi)[f(W,l,r)\cos\pi\delta_l - g(W,l,r)\sin\pi\delta_l]$$

$$W = -\frac{1}{2(n-\delta_l)^2}$$

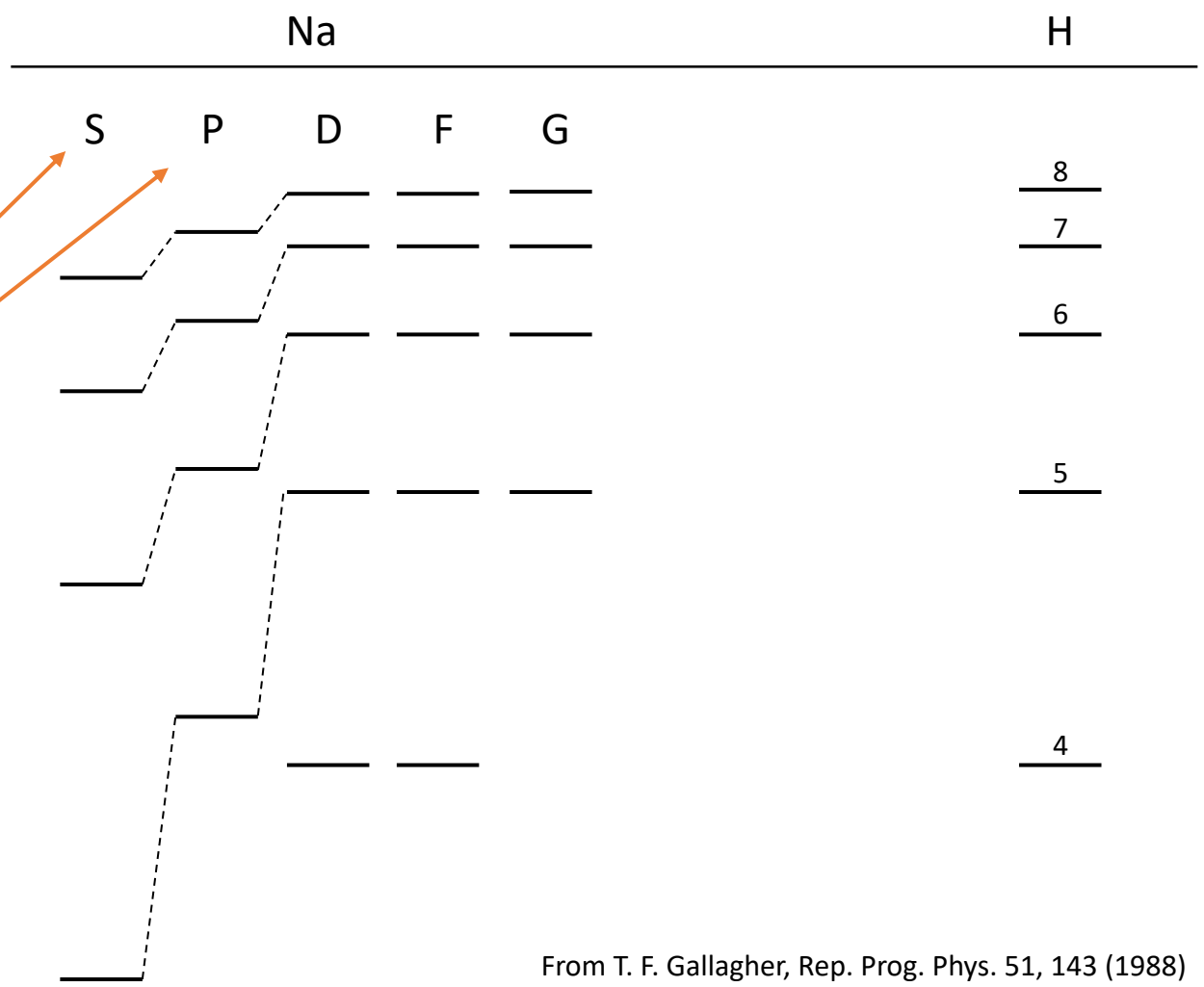
g functions no longer forbidden

To see the f and g functions: https://dlmf.nist.gov/33.3

Alkali metals

Difference in energy levels of H and Na

The δ_l defect is stronger for low angular momentum states



From T. F. Gallagher, Rep. Prog. Phys. 51, 143 (1988)

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Making qubits out of atoms

How do we make qubits out of this?

1- We need to identify a $|0\rangle$ and a $|1\rangle$ state

2- We need to be able to address transitions between $|0\rangle$ and $|1\rangle$

3- We need to know where the atoms are

4- We need to be able to produce entanglement between the atoms

5- We need to be able to measure the state of the system

Most of these are dependent on each other

Making qubits out of atoms

How do we make qubits out of this?

1- We need to identify a $|0\rangle$ and a $|1\rangle$ state

We use as a $|0\rangle$ the ground state of Rubidium:

$$1S^2\ 2S^2 2P^6 3S^2 3P^6 3D^{10} 4S^2 4P^6\ \underbrace{5S^1}$$

These are called Rydberg states

As a $|1\rangle$ state, we use a highly excited state, i.e. a state where the valence electron is in a level with high principal quantum number ($n \sim 70$)

$\|0\rangle \rightarrow \|5S\rangle$ $\|1\rangle \rightarrow \|60S\rangle$	$\|0\rangle \rightarrow \|5S\rangle$ $\|1\rangle \rightarrow \|70S\rangle$	$\|0\rangle \rightarrow \|5S\rangle$ $\|1\rangle \rightarrow \|70S\rangle$
https://arxiv.org/abs/2211.16337	https://arxiv.org/abs/2202.09372	https://arxiv.org/abs/1707.04344

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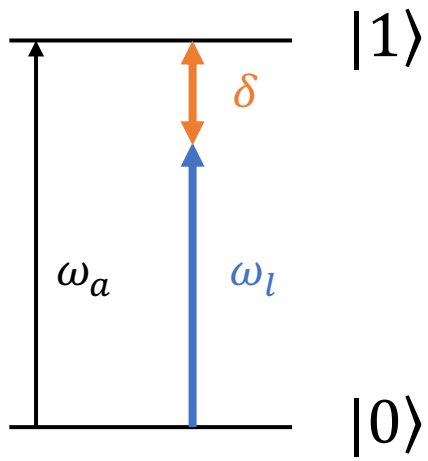
Making qubits out of atoms

How do we make qubits out of this?

2- We need to be able to address transitions between $|0\rangle$ and $|1\rangle$

This is done by shining on the atom a laser beam very close to the transition energy between $|0\rangle$ and $|1\rangle$

The difference between the resonant frequency ω_a and the laser frequency ω_l is called detuning, usually denoted δ



How do we make qubits out of this?

2- We need to be able to address transitions between $|0\rangle$ and $|1\rangle$

Sadly there's not enough time to go over the physics of the interaction between atom and light, but a good reference for that is the very first chapter of Metcalf, van der Straten – Laser Cooling and Trapping. It only requires QM knowledge.

The bottom line is that the system of valence electron coupled to light can be described by a simple two-level Hamiltonian:

$$H = \begin{bmatrix} -\delta & \Omega \\ \Omega & 0 \end{bmatrix}$$

- δ is the detuning of the laser
- Ω is the Rabi frequency, related to the intensity of the laser

Two-level systems like that have been studied first by Rabi, and they are solved in any standard quantum mechanics textbook. Solutions are oscillations between the state $|0\rangle$ and $|1\rangle$ (Rabi oscillations)

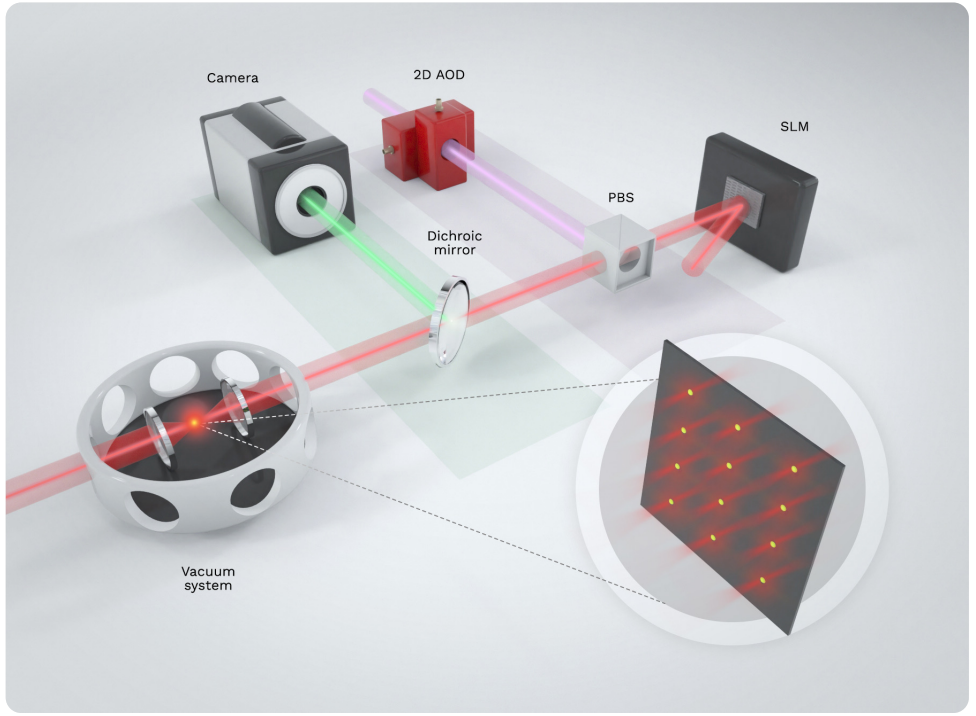
The frequency of the oscillations is given by $\sqrt{\Omega^2 + \delta^2}$, while the amplitude is maximum for resonant driving (zero detuning) and decreases with increasing detuning.

Making qubits out of atoms

How do we make qubits out of this?

3- We need to know where the atoms are

We use optical tweezers to trap individual atoms in a region of around 1 μm

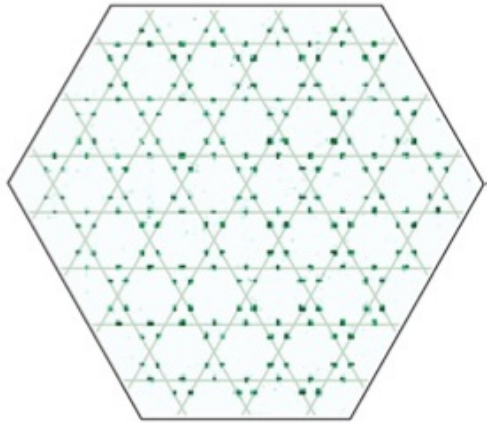


Making qubits out of atoms

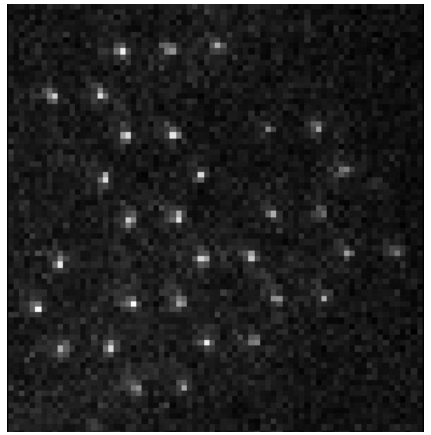
How do we make qubits out of this?

3- We need to know where the atoms are

High flexibility: atoms can be arranged in arbitrary fixed 2D configurations



https://arxiv.org/abs/2104.04119



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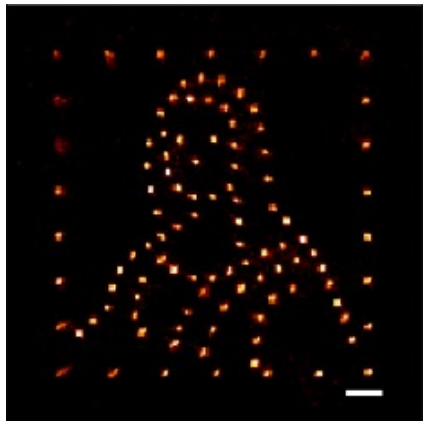

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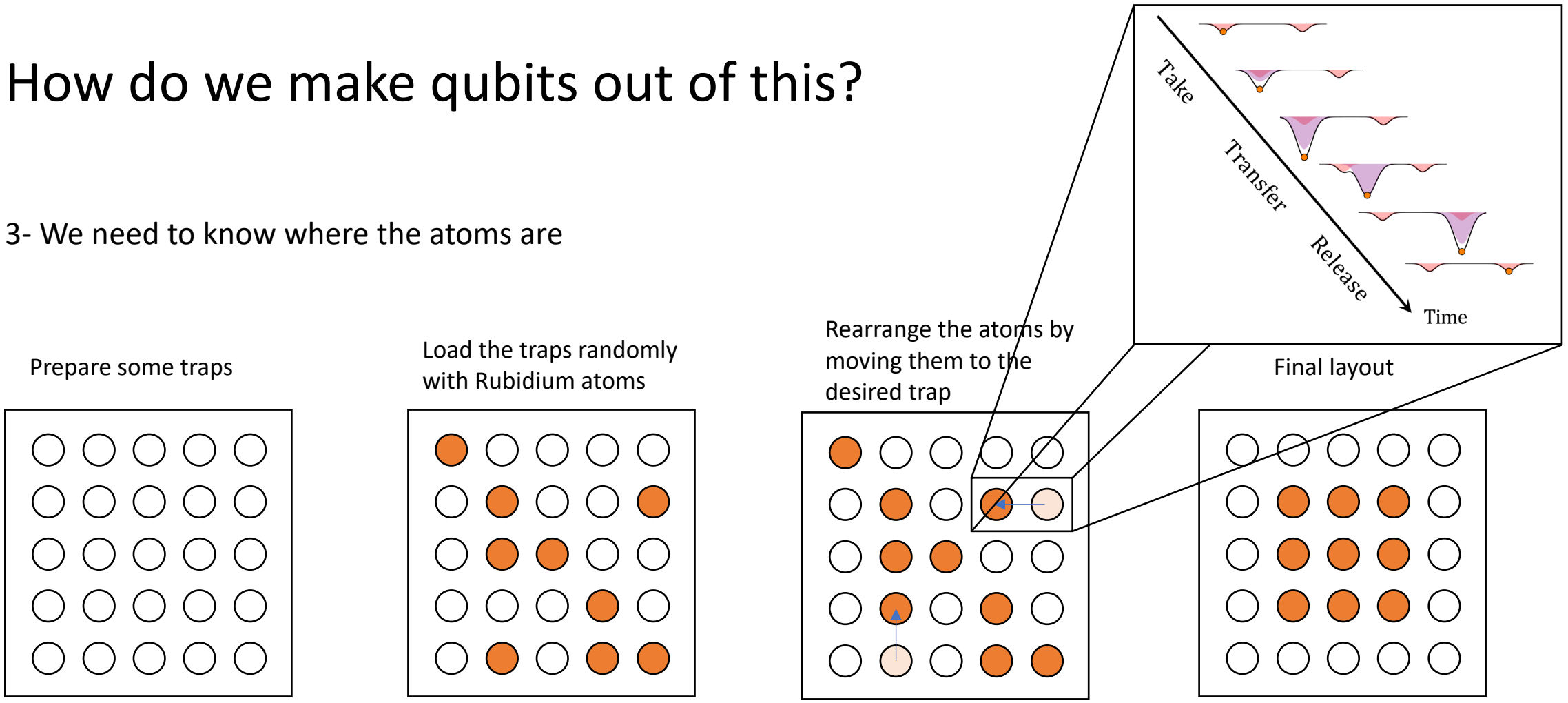
Making qubits out of atoms

How do we make qubits out of this?

3- We need to know where the atoms are



Making qubits out of atoms

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

We use what's called the *Rydberg blockade* mechanism

Making qubits out of atoms

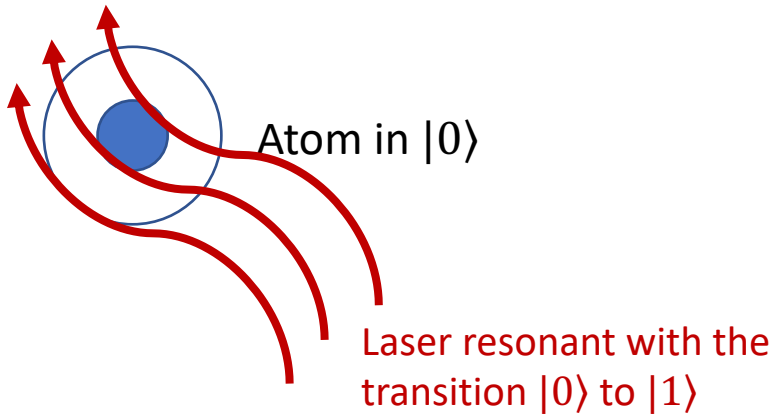
How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

Making qubits out of atoms

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms



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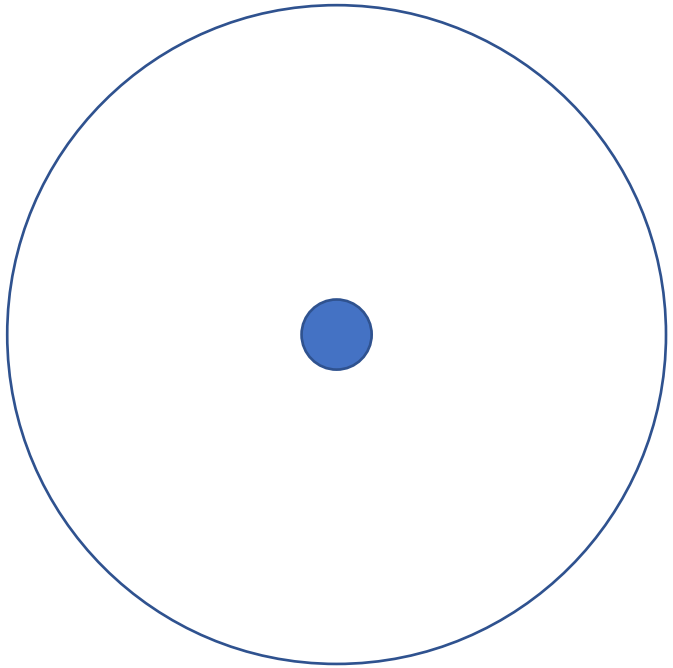
Making qubits out of atoms

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms



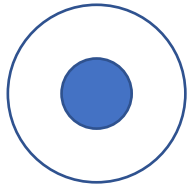
Atom in $|1\rangle$

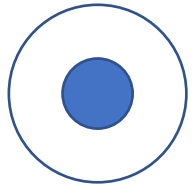
Making qubits out of atoms

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

Now two atoms in $|00\rangle$, far apart from each other ($\gtrsim 15\ \mu m$)

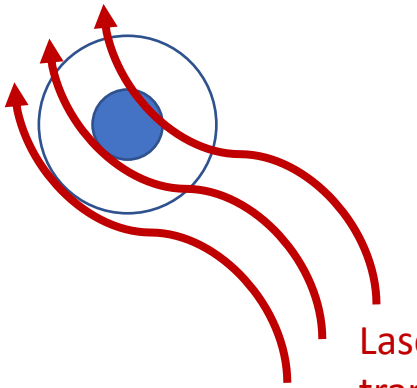




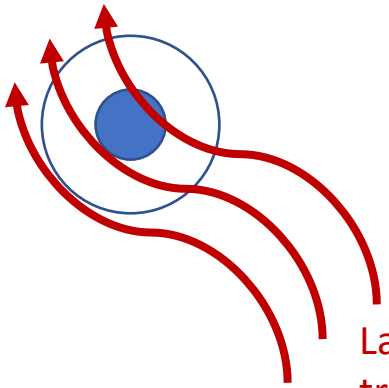
How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

Now two atoms in $|00\rangle$, far apart from each other ($\gtrsim 15\ \mu m$)
Shine resonant laser



Laser resonant with the transition $|0\rangle$ to $|1\rangle$



Laser resonant with the transition $|0\rangle$ to $|1\rangle$

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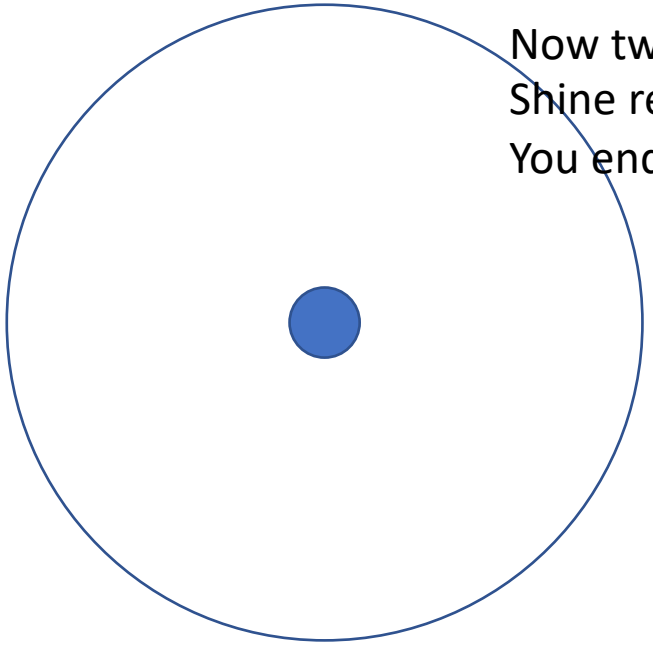
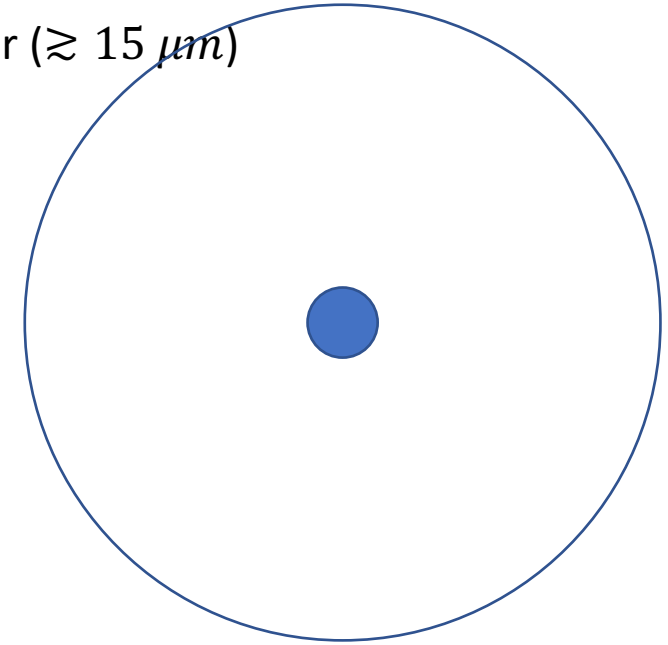
Making qubits out of atoms

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms



Now two atoms in $|00\rangle$, far apart from each other ($\gtrsim 15\ \mu m$)
Shine resonant laser
You end up with two excited atoms, $|11\rangle$



Making qubits out of atoms

How do we make qubits out of this?

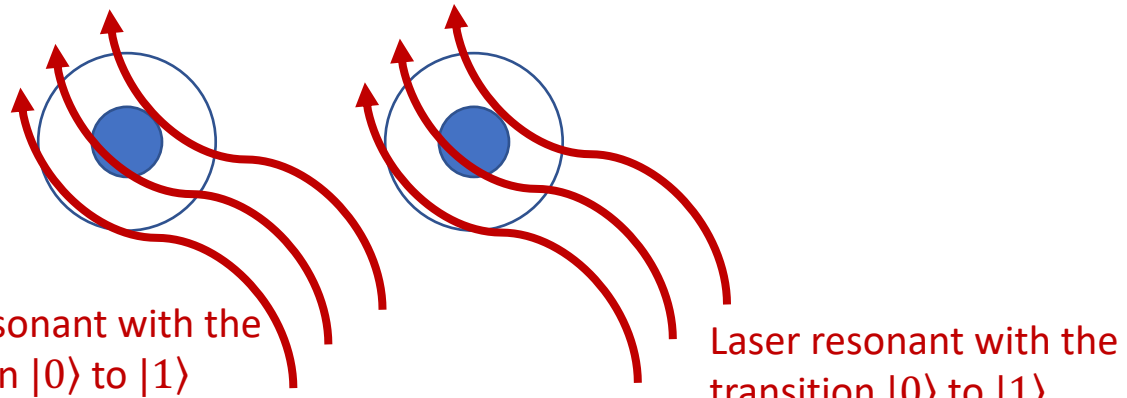
4- We need to be able to produce entanglement between the atoms

Now two atoms in $|00\rangle$, but close to each other (around $5-6\ \mu m$)

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

Now two atoms in $|00\rangle$, but close to each other (around $5-6\ \mu m$)
Shine resonant laser



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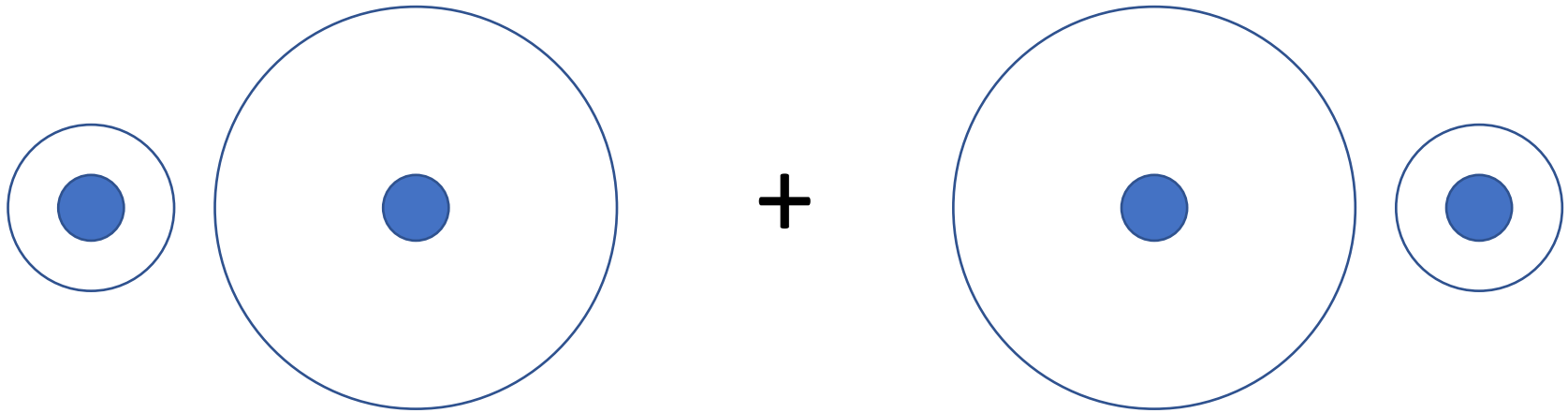
Making qubits out of atoms

How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

Now two atoms in $|00\rangle$, but close to each other (around $5-6\ \mu m$)
Shine resonant laser
You end up with the entangled state $|01\rangle + |10\rangle$ rather than $|11\rangle$



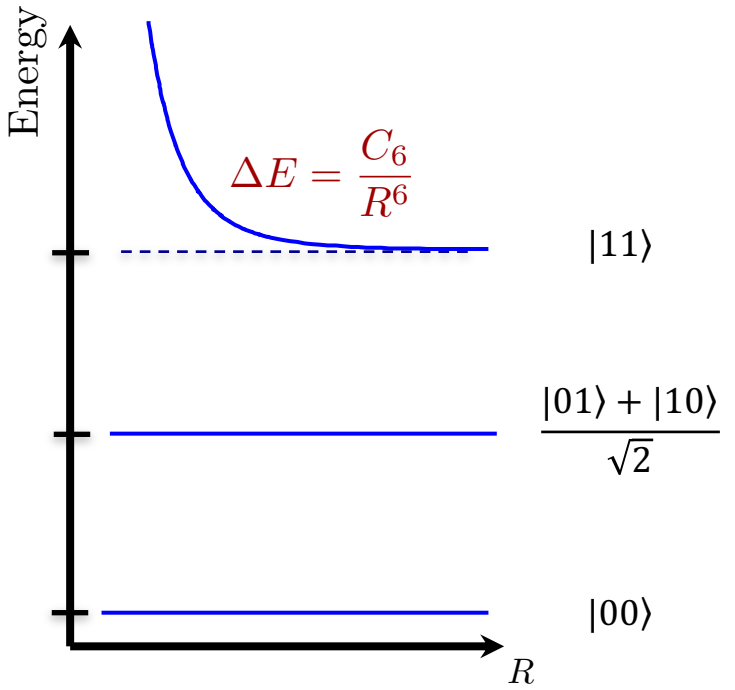
How do we make qubits out of this?

4- We need to be able to produce entanglement between the atoms

What's the physics behind the Rydberg blockade?

Two Rydberg states interact with a van der Waals interaction decaying as R^{-6} (with R distance between the atoms)

The interaction shifts upwards the energy of the $|11\rangle$ level, favouring the excitation of the entangled state $|01\rangle + |10\rangle$ instead



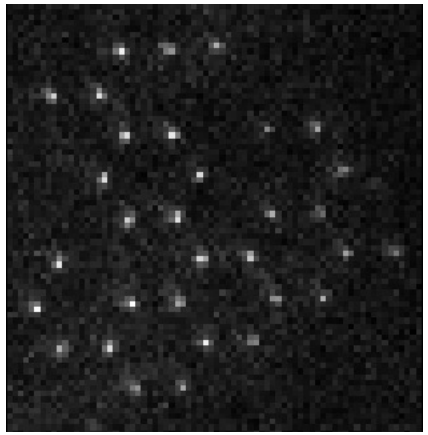
How do we make qubits out of this?

5- We need to be able to measure the state of the system

The optical tweezer is actually repulsive for atoms in the $|1\rangle$ state and for that reason, during quantum computations, the tweezers are switched off

So, after the quantum evolution of the system, the tweezers are turned back on and atoms in $|1\rangle$ are expelled from the traps and lost, while atoms in $|0\rangle$ are recaptured

Fluorescent light is shone on the atoms, and the emission is captured by a CCD camera, which therefore only sees atoms in $|0\rangle$. The remaining spots are then assumed to be atoms in the state $|1\rangle$.



https://arxiv.org/abs/2211.16337

Recap

1- We need to identify a $|0\rangle$ and a $|1\rangle$ state: Ground state and Rydberg state of Rubidium

2- We need to be able to address transitions between $|0\rangle$ and $|1\rangle$: Laser beams

3- We need to know where the atoms are: Optical tweezers

4- We need to be able to produce entanglement between the atoms: Rydberg blockade

5- We need to be able to measure the state of the system: Fluorescence imaging

Analog quantum computing with neutral atoms

Putting together all the ingredients we have seen so far, we can say this:

We are able to control systems of neutral atoms placed in fixed positions and interacting as dipoles

The Hamiltonian of a system of N atoms is the following:

$$\hat{H} = \sum_{i=1}^{N} \Omega_i \hat{\sigma}_i^x - \sum_{i=1}^{N} \delta_i \hat{n}_i + \sum_{i<j=1}^{N} \frac{C_6}{r_{ij}^6} \hat{n}_i \hat{n}_j$$

Ω = Rabi frequency

δ = Detuning

Analog quantum computing with neutral atoms

$$\sum_{i=1}^{N} \Omega_i \hat{\sigma}_i^x - \sum_{i=1}^{N} \delta_i \hat{n}_i$$

$$\hat{\sigma}_i^x = \hat{\mathbb{I}} \otimes \cdots \otimes \hat{\sigma}^x \otimes \cdots \otimes \hat{\mathbb{I}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

2x2 identity

Pauli x matrix in the i-th position

$$\hat{n}_i = \hat{\mathbb{I}} \otimes \cdots \otimes \hat{n} \otimes \cdots \otimes \hat{\mathbb{I}} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Number operator in the i-th position

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Analog quantum computing with neutral atoms

Where does it come from?

$$\sum_{i=1}^{N} \Omega_i \hat{\sigma}_i^x - \sum_{i=1}^{N} \delta_i \hat{n}_i$$

Take just one atom and recall the Hamiltonian for interaction between valence electron and light (slide 12):

$$H = \begin{bmatrix} -\delta & \Omega \\ \Omega & 0 \end{bmatrix}$$

This can be decomposed in terms of σ^x and n:

$$H = \begin{bmatrix} -\delta & \Omega \\ \Omega & 0 \end{bmatrix} = \Omega\, \hat{\sigma}^x - \delta\, \hat{n}$$

So the first part of the total Hamiltonian simply represents the interaction between the N atoms and the laser source

Analog quantum computing with neutral atoms

$$\sum_{i<j=1}^{N} \frac{C_6}{r_{ij}^6} \hat{n}_i \hat{n}_j$$

r_{ij} = distance between atom i and j

C_6 = physical constant

The last part of the Hamiltonian represents the interactions between the atoms.

Recall (slide 26) that two atoms in the Rydberg state interact as dipoles, which gives rise to the phenomenon of the Rydberg blockade.

This terms accounts for all the possible interactions between pairs of atoms in the Rydberg state.

Analog quantum computing with neutral atoms

$$\hat{H} = \sum_{i=1}^{N} \Omega_i \hat{\sigma}_i^x - \sum_{i=1}^{N} \delta_i \hat{n}_i + \sum_{i<j=1}^{N} \frac{C_6}{r_{ij}^6} \hat{n}_i \hat{n}_j$$

- Positive detuning on one atom decreases the energy of the system (excitation is energetically favoured)

- Two excitations close to each other increase the energy of the system (close excitations are energetically disfavoured)

- It's a transverse field quantum Ising model, where the interaction strength depends on the distance between atoms

Solving combinatorial problems

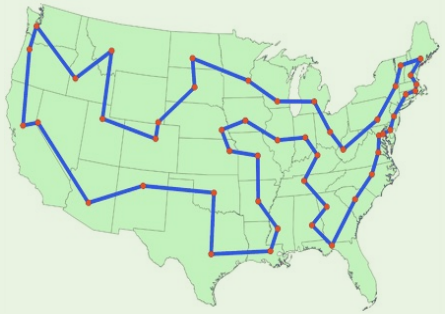
PASQAL

Quantum solver for combinatorial problems

Combinatorial Problems

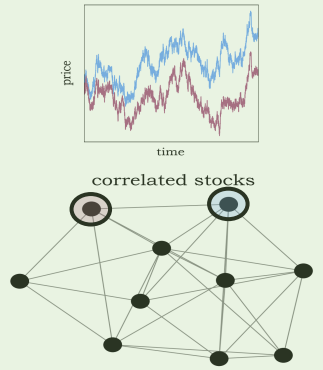
- Combinatorial optimization is at the heart of many real-world problems
  - It consists in finding the ***best*** out of a finite, but prohibitively large, set of options
  - They have been extensively studied by both academic and industrial communities
  - And have a vast range of applications in real-world systems.
  - Too many options to explore (exponentially large) !

Delivering



Find an itinerary which visits every location while minimizing total distance

Portfolio Optimization



Select the best stocks to invest

Quantum solver for combinatorial problems

Combinatorial problems and Graphs

- Combinatorial problems can naturally be defined on graphs
  - are data structures composed of a set of elements called ***vertices*** (also known as nodes)
    - they can potentially be connected
    - different labels and weights can also be associated with vertices in order to differentiate them
  - These connections are called **edges** and might potentially encode different information
    - importance of such connections (as weights)
    - the distance between their endpoints
  - Several real-world optimization problems, from a vast spectrum of fields, can be mapped to graph problems
    - social experiments , telecommunication networks, physical systems, …
    - logistics, resource allocation, risk management, job scheduling, portfolio management, …
  - The related optimization problems typically consist **in selecting a subset** of vertices and/or edges **optimally satisfying certain rules**.

Quantum solver for combinatorial problems

Combinatorial problems on Graphs and QUBO formulations

QUBO is an acronym for a Quadratic Unconstrained Binary Optimization problem

It can embrace an exceptional variety of important CO problems found in industry, science and government

The QUBO model is expressed by the optimization problem:

QUBO: maximize/minimize $\boldsymbol{x}^t\boldsymbol{Q}\boldsymbol{x}$

where $\boldsymbol{x}$ is a vector of **binary** decision variables and $\boldsymbol{Q}$ is a square matrix of **constants**.

$$\text{QUBO} = \begin{bmatrix} x_i & \cdots & x_j \end{bmatrix} \begin{bmatrix} Q_{ii} & \cdots & Q_{ij} \\ \vdots & \ddots & \vdots \\ Q_{ji} & \cdots & Q_{jj} \end{bmatrix} \begin{bmatrix} x_i \\ \vdots \\ x_j \end{bmatrix}$$

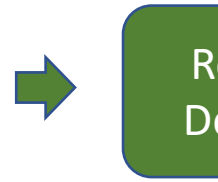
It is common to assume that the $\boldsymbol{Q}$ matrix is symmetric or in upper triangular form

Quantum solver for combinatorial problems

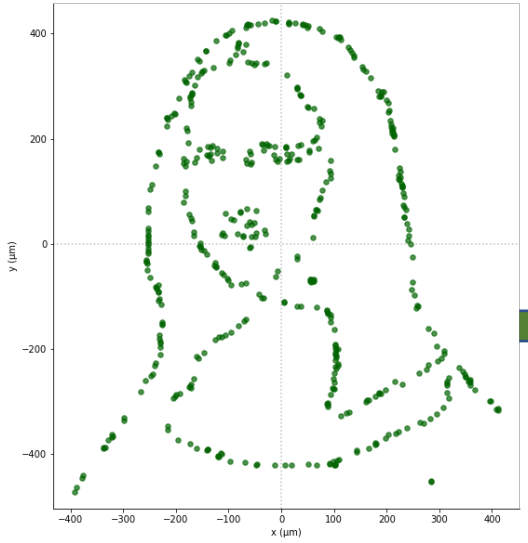
Creating a register for a given QUBO instance

- We now illustrate how to use Pulser to embed the QUBO matrix Q on a neutral-atom device.
- The key idea is to encode the off-diagonal terms of Q by using the Rydberg interaction between atoms.
  - The interaction U_{ij} depends on the pairwise distance ($U_{ij} = C_6/r_{ij}^6$) between atoms i and j.
    - C_6 is a constant given by the system/device, while r_{ij} is the distance between atoms i and j.
  - We attempt to find the optimal positions of the atoms in the Register that replicate best the off-diagonal terms of terms of Q.

$$Q = \begin{bmatrix} Q_{ii} & \cdots & Q_{ij} \\ \vdots & \ddots & \vdots \\ Q_{ji} & \cdots & Q_{jj} \end{bmatrix}$$



Register Designer



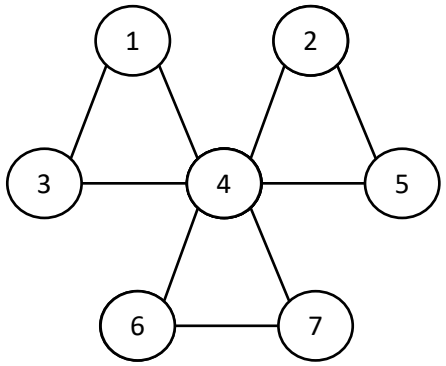
$$U = \begin{bmatrix} U_{ii} & \cdots & U_{ij} \\ \vdots & \ddots & \vdots \\ U_{ji} & \cdots & U_{jj} \end{bmatrix}$$

PASQAL

Quantum solver for combinatorial problems

An **independent set (IS)** of a graph G is a subset of the vertices such that no two vertices in the subset represent an edge of G.

A maximum independent set (MIS) is a vertex set containing the largest possible number of vertices for a given graph.



$$QUBO_{MIS} = \sum_{i \in V} x_i - \sum_{(i,j) \in E} 2 x_i x_j$$

$$\begin{bmatrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 0 & 1 & -1 & 0 & 0 & 0 \\ -1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 0 & -1 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{bmatrix} = ?$$

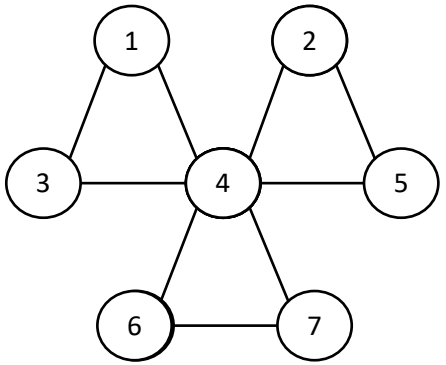
$QUBO_{MIS}$ (G)

$$\begin{aligned} \max \quad & x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 \\ & - 2\, x_4 (x_3 + x_5 + x_6 + x_7) \\ & - 2\, x_1 (x_3 + x_4) \\ & - 2\, x_2 (x_4 + x_5) \\ & - 2\, x_6 x_7 \end{aligned}$$

$$\begin{aligned} \min \quad & -x_1 - x_2 - x_3 - x_4 - x_5 - x_6 - x_7 \\ & + 2\, x_4 (x_3 + x_5 + x_6 + x_7) \\ & + 2\, x_1 (x_3 + x_4) \\ & + 2\, x_2 (x_4 + x_5) \\ & + 2\, x_6 x_7 \end{aligned}$$

PASQAL

Quantum solver for combinatorial problems



$QUBO_{MIS}$

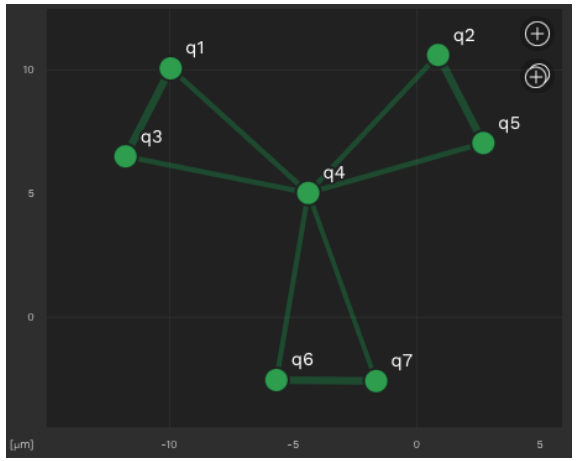
$$\begin{bmatrix} 1 & 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 0 & 1 & -1 & 0 & 0 & 0 \\ -1 & -1 & -1 & 1 & -1 & -1 & -1 \\ 0 & -1 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 & 0 & -1 & 1 \end{bmatrix}$$

Each atom represents a node on the graph

Two atoms are put **close** to each other if their related nodes **are connected** by a link (or if $Q_{ij} < 0$)

Two atoms are put **far from each** other if their related nodes **are <u>not</u> connected** by a link (or if $Q_{ij} \geq 0$)

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



$$U = \begin{bmatrix} -15 & 4.5 & 1197 & 30 & 0.8 & 0.9 & 0.5 \\ & -15 & 1.3 & 49 & 1323 & 0.7 & 1.5 \\ & & -15 & 29 & 0.4 & 3.2 & 0.9 \\ & & & -15 & 15 & 26 & 24 \\ & & & & -15 & 0.8 & 2.6 \\ & & & & & -15 & 1323 \\ & & & & & & -15 \end{bmatrix}$$

PASQAL

Quantum solver for combinatorial problems

The Quantum Adiabatic Algorithm

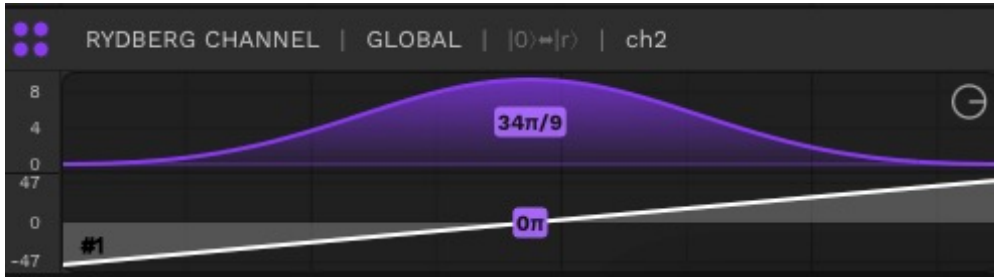
- The idea behind the adiabatic algorithm is to slowly evolve the system from an easy-to-prepare ground-state to the ground-state of H_Q.
  - If done slowly enough, the system of atoms stays in the instantaneous ground-state.

- We continuously vary the parameters Ω(t),δ(t) in time
  - starting with $\boldsymbol{\Omega_{t_0} = 0}$ and $\boldsymbol{\delta_{t_0} < 0}$
  - ending with $\boldsymbol{\Omega_{t_f} = 0}$ and $\boldsymbol{\delta_{t_f} > 0}$

- The ground-state of $\boldsymbol{H_{t_0}}$ corresponds to the initial state **|00000⟩** and the ground-state of $\boldsymbol{H_{t_f}}$ corresponds to the ground-state **of** $\boldsymbol{H_Q}$.

- The Rydberg blockade radius is directly linked to the Rabi frequency **Ω**

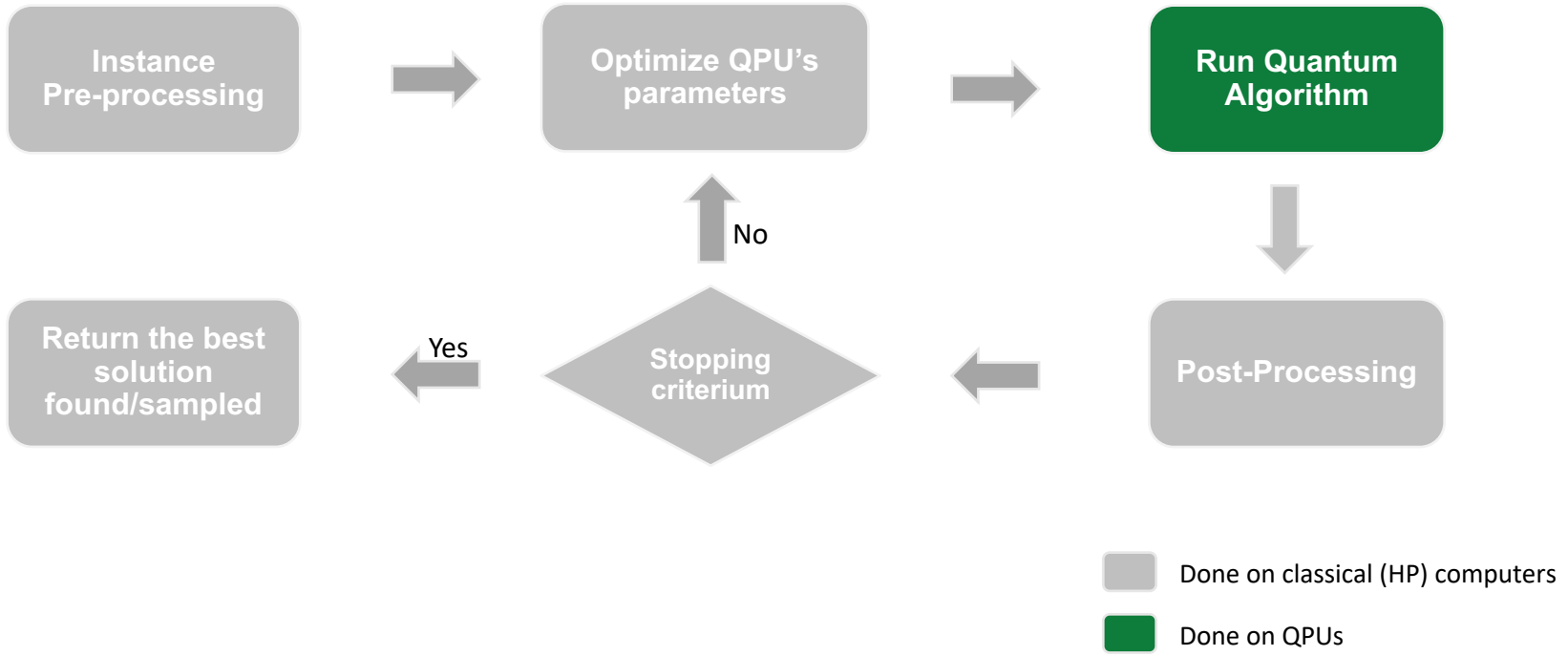
- We can therefore build the adjacency matrix of the input G in the following way
  - To ensure that we are not exciting the system to states that are too excited, we keep $\boldsymbol{\Omega_{max}} \in \left[\boldsymbol{\Omega_{disjoint}}, \boldsymbol{\Omega_{connected}}\right]$
    - set $\boldsymbol{\Omega_{disjoint}} = \mathrm{argm}ax_{(i,j)\notin E}\ \mathrm{U_{ij}}$
    - set $\boldsymbol{\Omega_{connected}} = \mathrm{argm}in_{(i,j)\in E}\ \mathrm{U_{ij}}$



Quantum solver for combinatorial problems

What if we don’t know what the QUBO matrix represents ?

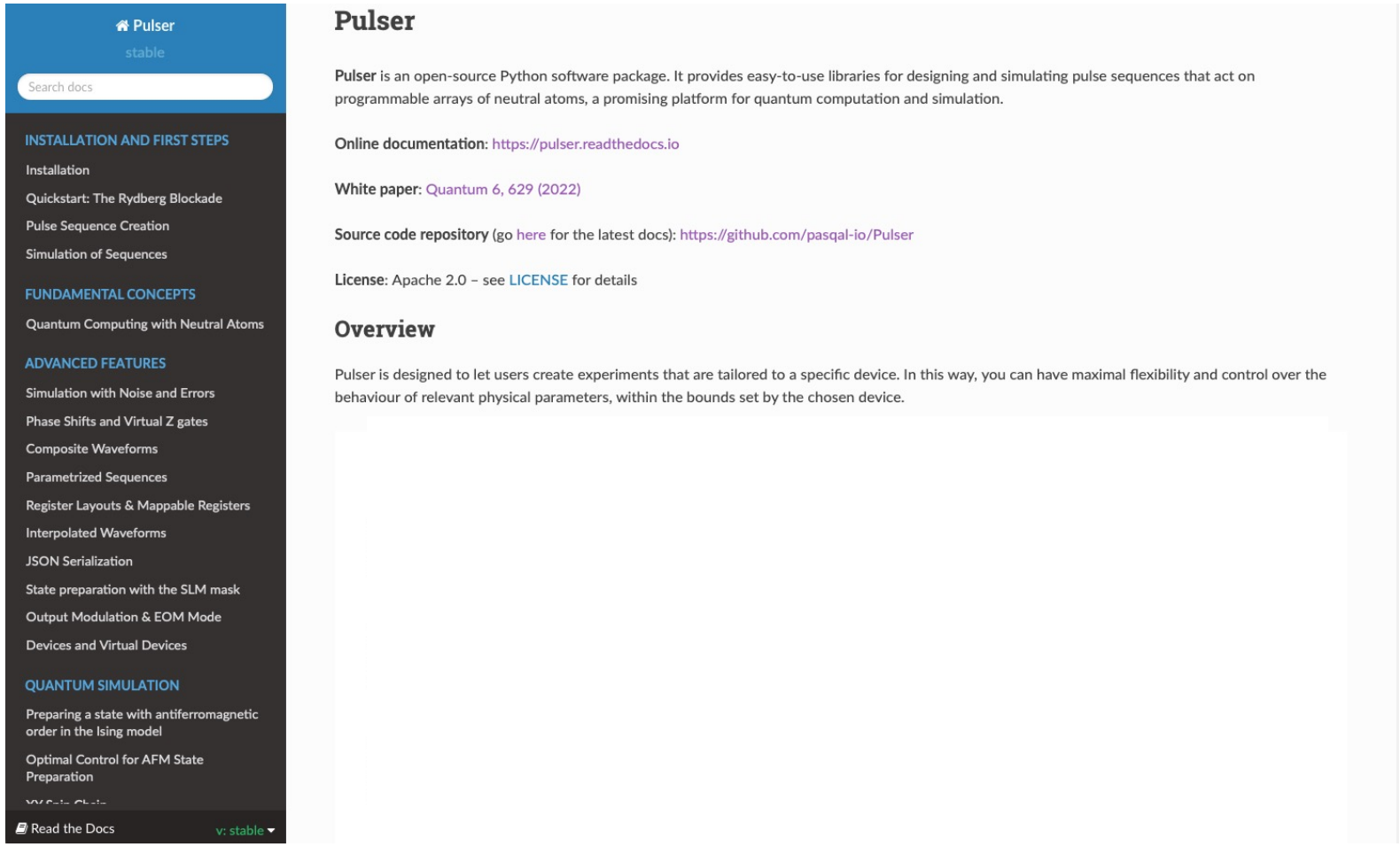
- CPUs and QPUs can be coupled to solve optimization problems
- Many QC algorithms involve classical pre- or post-processing
- Many of them also include close-loop optimization



Quantum solver for combinatorial problems

For more complex algorithms, try Pulser

Pulser is an open-source Python software package. It provides easy-to-use libraries for designing and simulating pulse sequences that act on programmable arrays of neutral atoms, a promising platform for quantum computation and simulation.



Thank you

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