Quantum solutions for energy and environmental challenges

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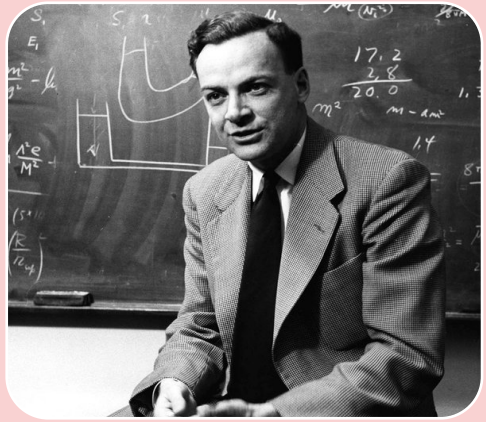
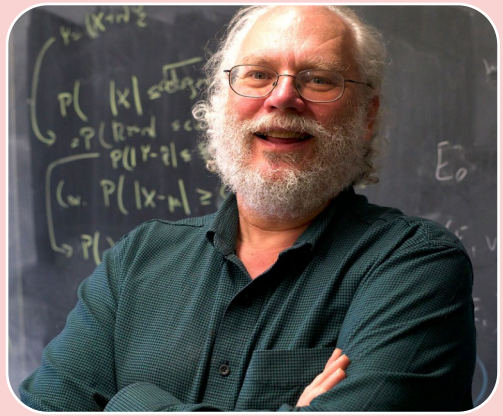
Quantum computation



1981

Feynman (Caltech)

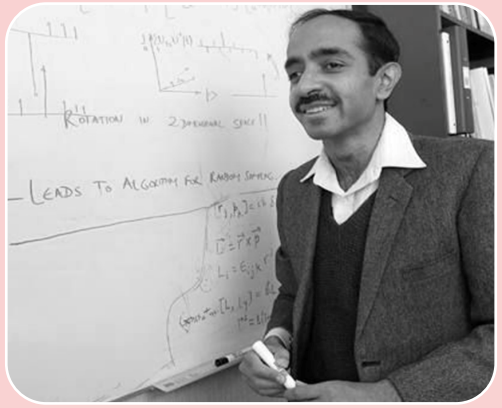
Simulate quantum systems efficiently



1994

Shor(AT&T Labs)

Exponential speed up-factoring large numbers



1996

Grover (Bell Labs)

Quadratic speed up -unstructured search

2009

Harrow-Hassidim-Lloyd (MIT)

Exponential speed up-linear systems

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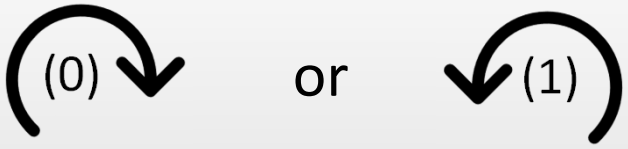
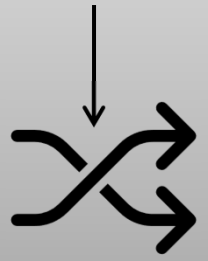
Quantum computation (superposition)

Classical bit: fundamental unit of classical information, having a value of either 0 or 1.



Electric current

Quantum bit: the basic unit of quantum information, capable of existing in superposition.

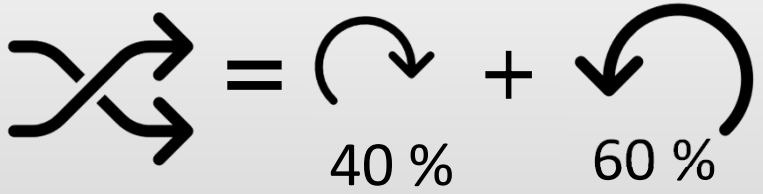


State	CW %	CCW%
1	100	0
2	0	100
3	40	60

Countless possibilities for qubit state!!

Probability interpretation

State of the qubit (superposition)



$$|\Psi\rangle = \sqrt{0.4}|0\rangle + \sqrt{0.6}|1\rangle$$

$$\text{CW: } 0 \rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \equiv |0\rangle$$

$$\text{CCW: } 1 \rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv |1\rangle$$

Ket notation

Four qubit (16 d vector)

$$|0000\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Quantum computation (entanglement)

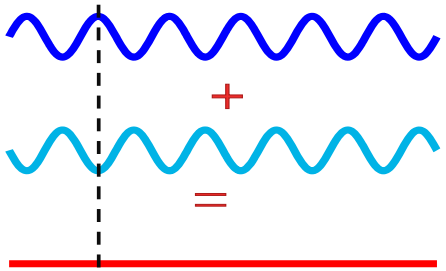
+

Entangled coins: two coins, held by individuals on Earth and the Moon, are connected in such a way that observing one coin instantly determines the state of the other.

Quantum computation (interference)

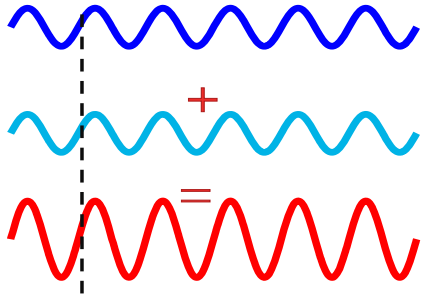
How does it work?

Destructive interference

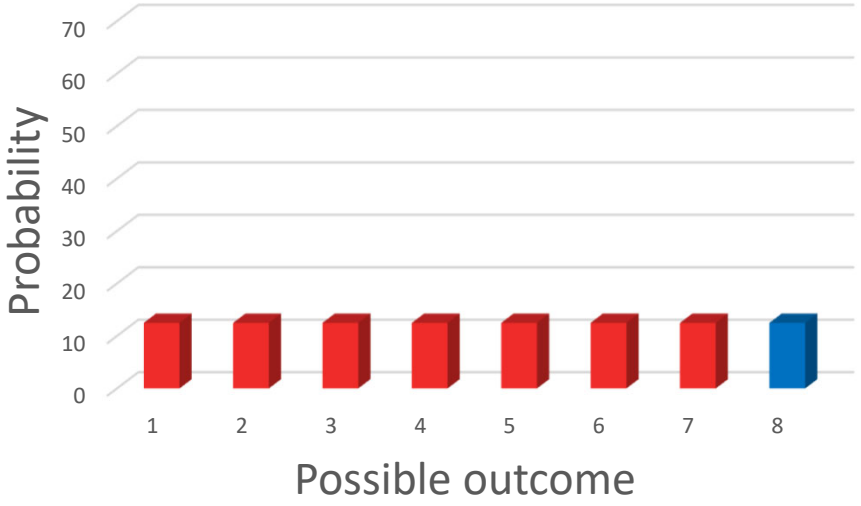


To diminish the probability of obtaining the incorrect answers

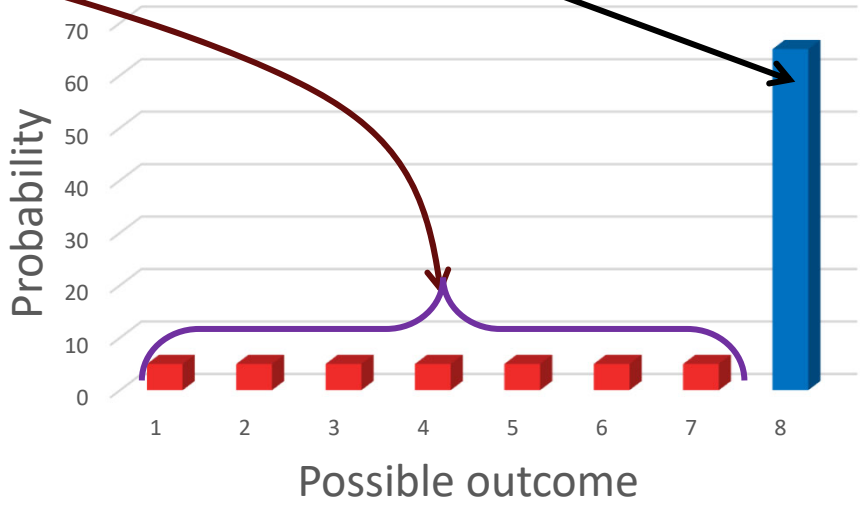
Constructive interference



To amplify the probability of obtaining the correct answer



Interference



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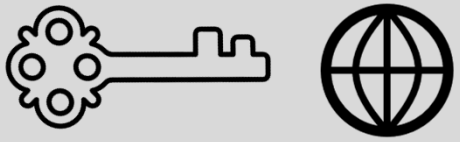
Quantum computation power

How hard is prime factorization and why it is important?

Easy computation (multiplication) used for encryption

$7212277 \times 5040533 = 36353720223641$

Difficult computation (factoring) is needed for decryption



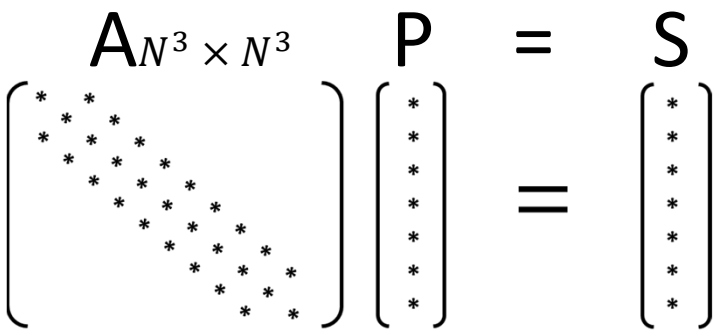
RSA decryption:

Hardness of factoring a very large number (600-digit)

- Quantum computer can break RSA exponentially faster than classical computers **(Shor algorithm)**
- **Theory:** approximately 4000 qubits to factorize this number
- **In practice:** 4,000,000 qubits due to error correction

Quantum computing for seismic modeling

Quantum linear system solver for seismic wave modeling



Discretization

3D wave equation

$$\left(-\nabla^2 - \frac{\omega^2}{c^2(\mathbf{x})}\right) p(\mathbf{x}, \omega) = s(\mathbf{x}, \omega)$$

Complexity

Harrow, **H**assidim, **L**loyd, 2009. PRL.

Quantum	Classical
$O(\kappa \log N)$	$O(\kappa N^3)$

κ: condition number of matrix A

Complexity

S. Moradi et al, CJEG, 2019

Quantum	Classical
$O(N^2 \log N)$	$O(N^5)$

$\kappa = N^2$

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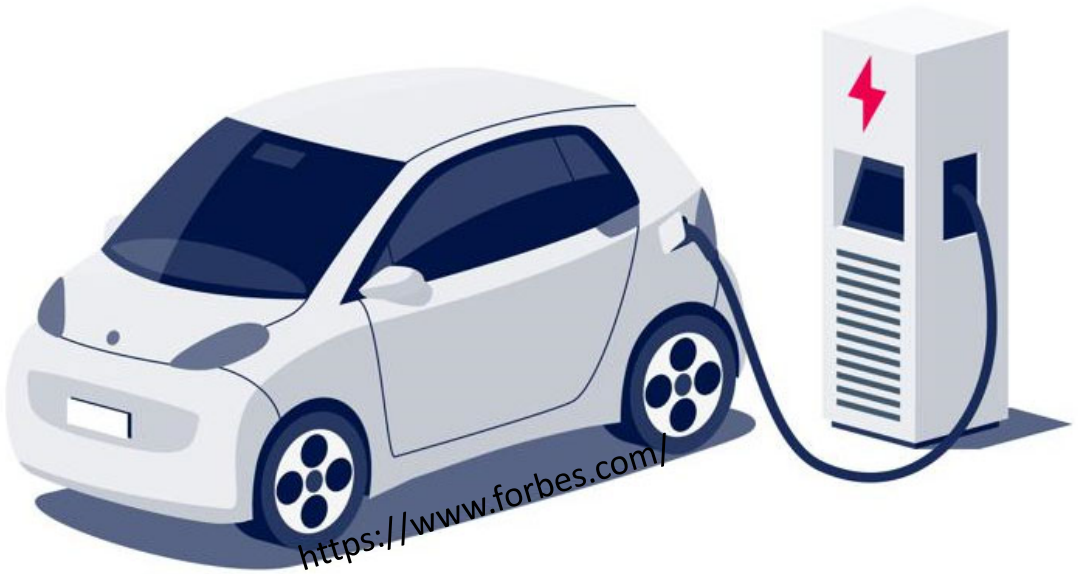
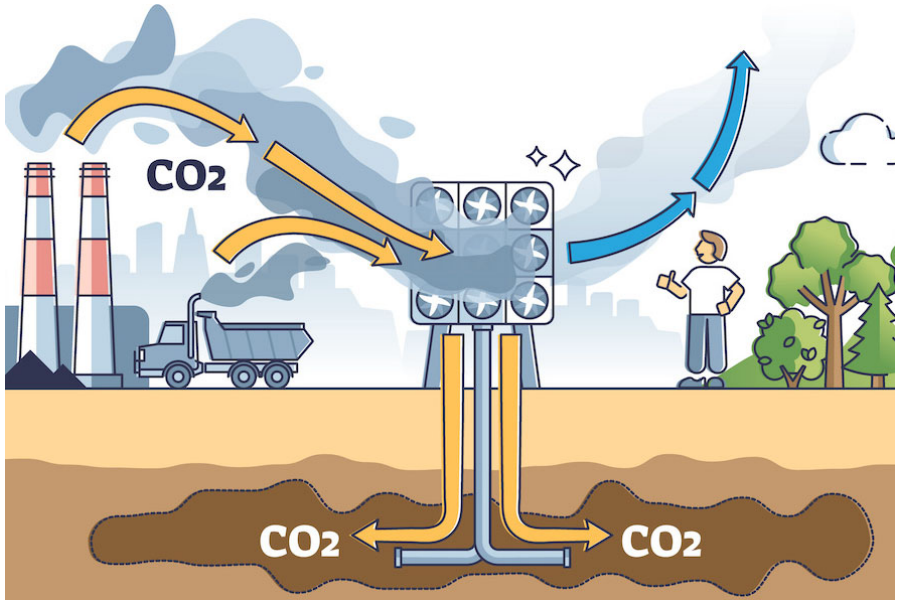
Quantum computing for energy

Quantum algorithm for battery simulation



https://www.forbes.com/

Quantum algorithms for carbon capture strategies



https://www.resourceworks.com/

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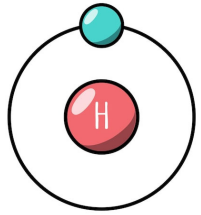
Quantum computing for chemistry

Hydrogen atom (one electron)



$$\left[-\frac{\hbar^2}{2m_p}\nabla_p^2 - \frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{e^2}{|\vec{r}_e - \vec{r}_p|}\right]\chi(\vec{r}_e, \vec{r}_p) = E\,\chi(\vec{r}_e, \vec{r}_p)$$

Energy level

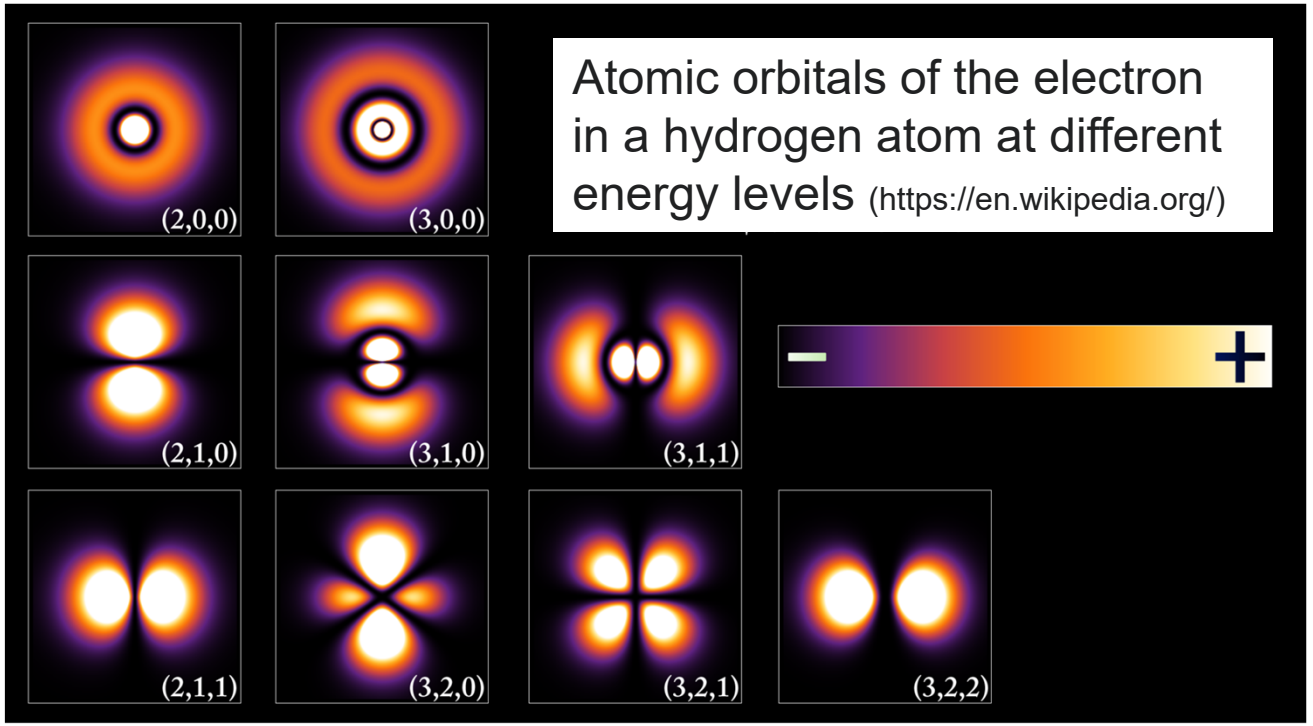
Excited state

3rd — $E_4 = -0.85$ eV

2nd — $E_3 = -1.51$ eV

1st — $E_2 = -3.4$ eV

Ground state — $E_1 = -13.6$ eV



Atomic orbitals of the electron in a hydrogen atom at different energy levels (https://en.wikipedia.org/)

Number of configurations $C_N^m \approx \frac{N^m}{m!}$

Number of orbitals

Number of electrons

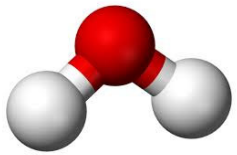
Chromium molecule

$C_{30}^{48} \approx 10^9$

Quantum computing for chemistry

Variational Quantum Eigensolver (VQE)

Hamiltonian encoding



Writing Hamiltonian (H) in terms of Pauli operators

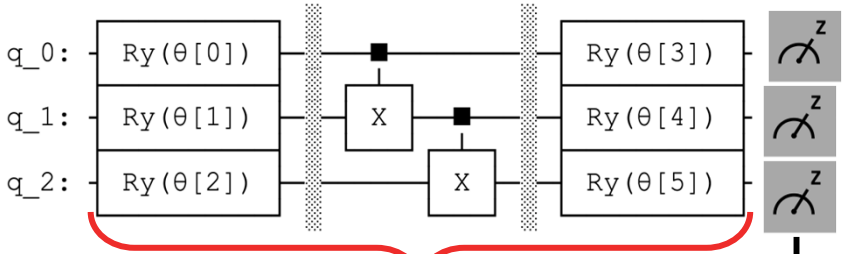
$$\hat{H} = \sum_i \alpha_i \hat{P}_i$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$X \otimes \mathrm{Y} \otimes \mathrm{Z} \otimes Z$$
$$Z \otimes \mathrm{Y} \otimes \mathrm{X} \otimes Z$$
$$Y \otimes \mathrm{Z} \otimes \mathrm{Z} \otimes X$$

Quantum computer

Ansatz and state preparation



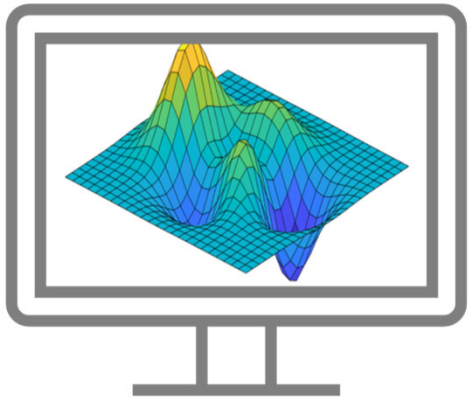
$$|\psi(\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5)\rangle$$

Measurement

$$E(\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5) = \left\langle \psi\left(\vec{\theta}\right) \middle| H \middle| \psi\left(\vec{\theta}\right) \right\rangle$$

Updated parameters

Classical computer



Optimization

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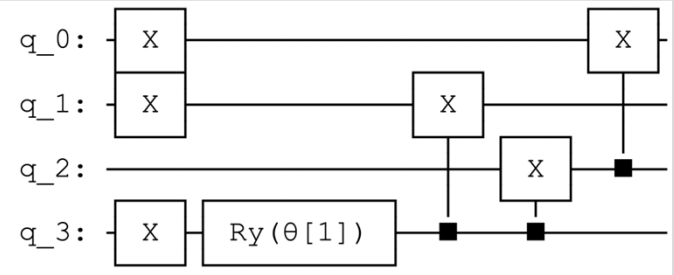
Quantum computing for chemistry

The ground state energy of the hydrogen molecule H_2

https://pennylane.ai

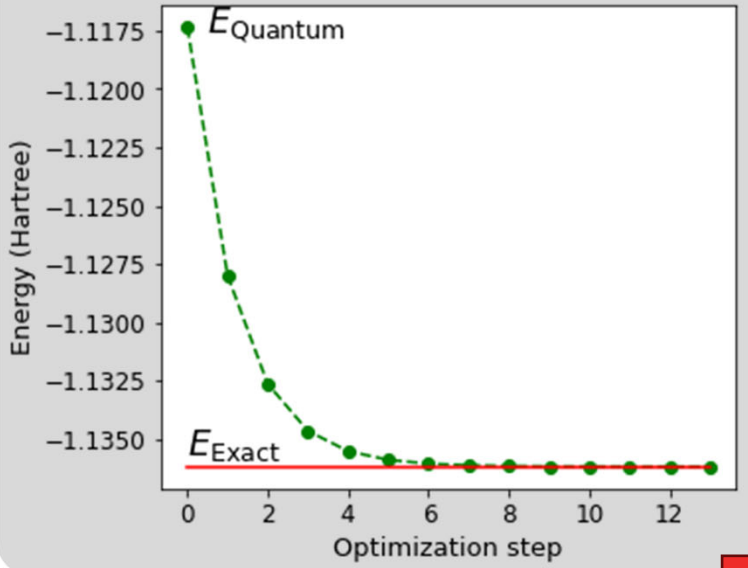
Quantum circuit

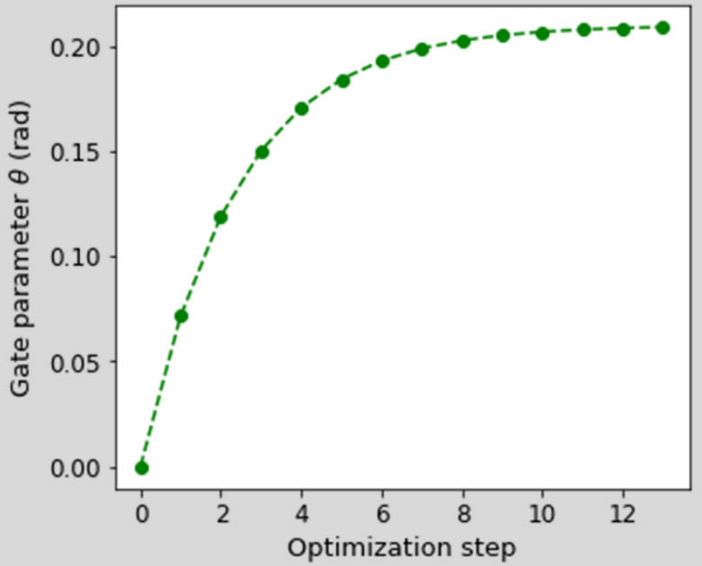


$$|\psi(\theta)\rangle = \cos(\theta)\,|1100\rangle - \sin(\theta)\,|0011\rangle$$

Optimization

$$E(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$$





$$|\psi(0.208)\rangle = 0.994|1100\rangle - 0.104|0011\rangle$$

Hamiltonian for molecule H_2

$$H = -(0.2427450126098118)I \otimes I \otimes Z \otimes I - (0.2427450126098118)I \otimes I \otimes I \otimes Z + \cdots + (0.044750084063064466)\,X \otimes Y \otimes Y \otimes X$$

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Conclusions: quantum landscape

- **Seismic modeling and inversion:**
  Algorithm: significant speed-up not attainable with classical computers.
  Implementation: requires a fault-tolerant quantum computer (>10 yrs.)
- **Quantum chemistry, battery design, and CCUS:**
  Algorithm: exploring hybrid solvers, such as VQE.
  Implementation: on noisy quantum devices with a few thousand qubits (< 5 yrs.)
- **Quantum computation in Canada:** National Quantum Strategy:
  - $139 billion industry
  - 200,000 jobs
  - $42 billion in returns by 2045.
- **Quantum computation in Calgary:**
  - Transformation of Calgary into a quantum city.
  - Leadership of University of Calgary's in advancing quantum science and technology.

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Professional Masters in Quantum Computing

2024

Launch year

20-25

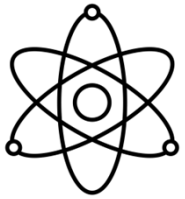
Person cohorts for small-group experience

3

Options – Certificate, Diploma, or Master's

Internship options for every student

Instructors are global leaders in their fields



Part of Alberta's nation-leading quantum ecosystem

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Thanks!

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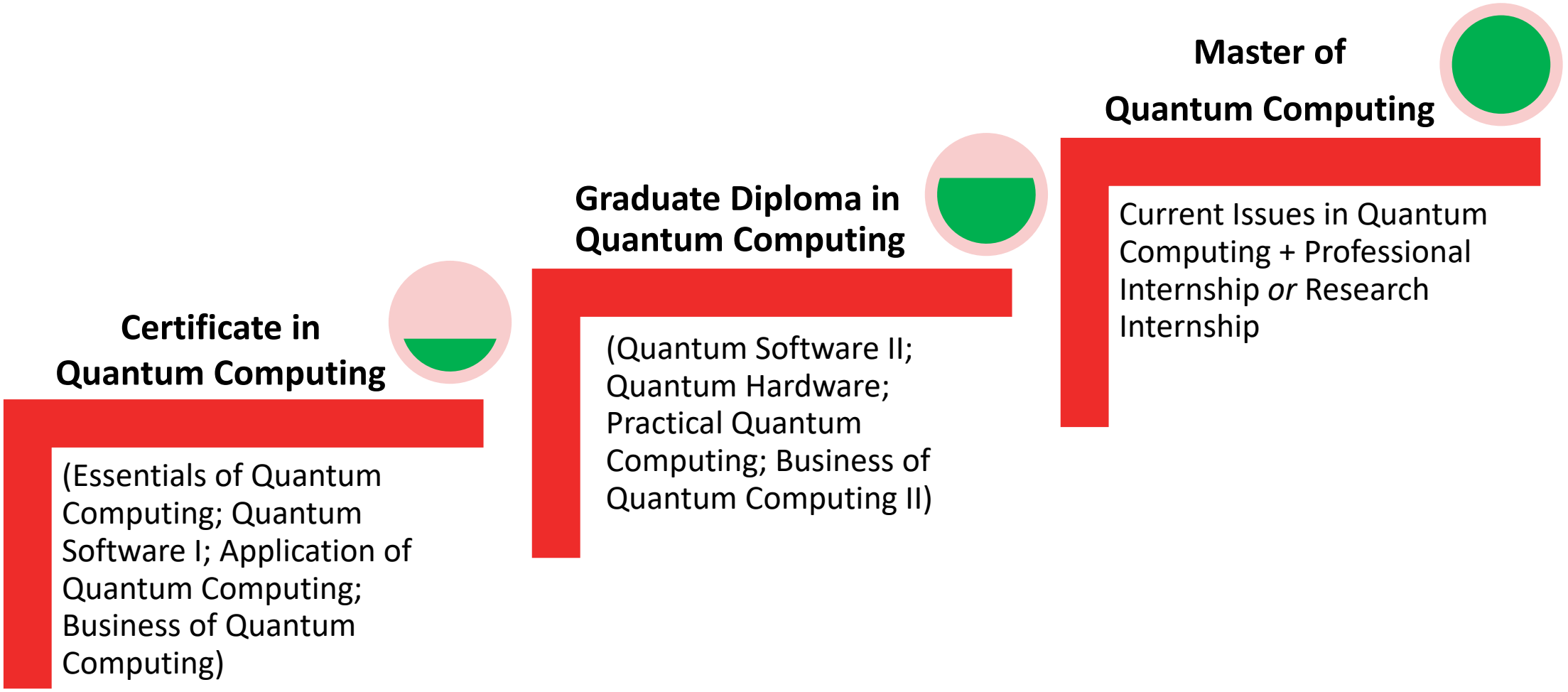
Professional Masters in Quantum Computing



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