Kvanteteknologi og kunstig intelligens

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Faglig pedagogisk dag, 31 2024

Kort oppsumering

Kvanteteknologi og kunstig intelligens er teknologier som vil kunne revolusjonere måten vi jobber og lever på og er forventa å kunne gi store fordeler for vitenskapelig og teknologisk utvikling, og vil sannsynligvis påvirke store og/eller alle deler av framtidas samfunn. Foredraget her vil ta for seg hvordan disse teknologiene vil påvirke naturfaglig og teknologisk forskning og undervisning, og hvorfor det er så viktig å forstå mulighetene og begrensningene.

Lysark finner du her `https://github.com/mhjensenseminars/MachineLearningTalk/tree/master/doc/pub/FPD`

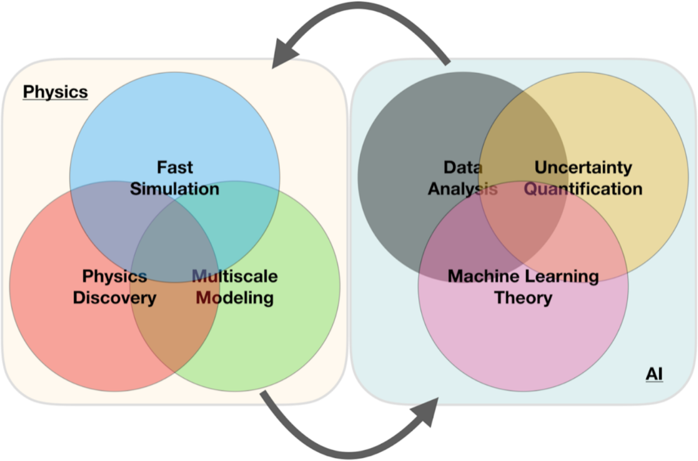
AI/ML and some statements you may have heard (and what do they mean?)

1. Fei-Fei Li on ImageNet: **map out the entire world of objects** (The data that transformed AI research)
2. Russell and Norvig in their popular textbook: **relevant to any intellectual task; it is truly a universal field** (Artificial Intelligence, A modern approach)
3. Woody Bledsoe puts it more bluntly: **in the long run, AI is the only science** (quoted in Pamilla McCorduck, Machines who think)

If you wish to have a critical read on AI/ML from a societal point of view, see Kate Crawford's recent text Atlas of AI.

Here: with AI/ML we intend a collection of machine learning methods with an emphasis on statistical learning and data analysis

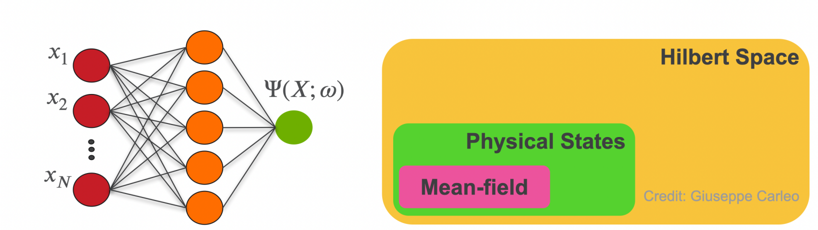
Machine learning. A simple perspective on the interface between ML and Physics



Neural network quantum states

Neural networks compactly represent complex high-dimensional functions

Most quantum states of interest have distinctive features and intrinsic structures



Types of machine learning

The approaches to machine learning are many, but are often split into two main categories. In *supervised learning* we know the answer to a problem, and let the computer deduce the logic behind it. On the other hand, *unsupervised learning* is a method for finding patterns and relationship in data sets without any prior knowledge of the system.
An important third category is *reinforcement learning*. This is a paradigm of learning inspired by behavioural psychology, where learning is achieved by trial-and-error, solely from rewards and punishment.

Main categories

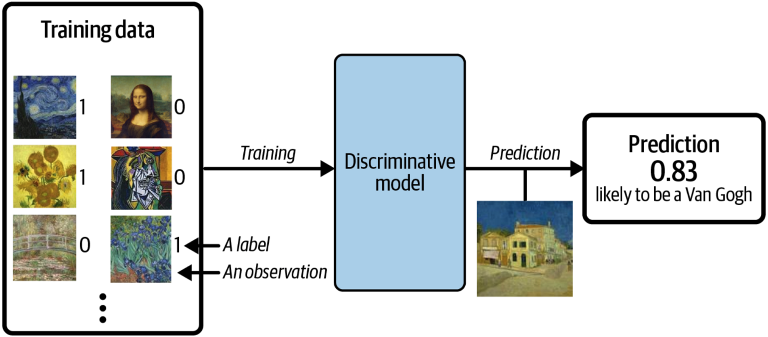
Another way to categorize machine learning tasks is to consider the desired output of a system. Some of the most common tasks are:

- Classification: Outputs are divided into two or more classes. The goal is to produce a model that assigns inputs into one of these classes. An example is to identify digits based on pictures of hand-written ones. Classification is typically supervised learning.
- Regression: Finding a functional relationship between an input data set and a reference data set. The goal is to construct a function that maps input data to continuous output values.
- Clustering: Data are divided into groups with certain common traits, without knowing the different groups beforehand. It is thus a form of unsupervised learning.

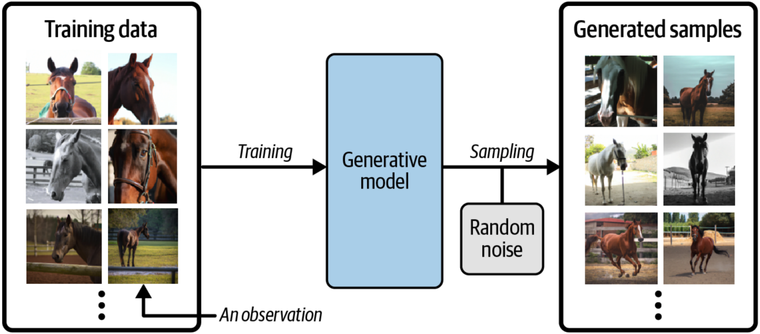
The plethora of machine learning algorithms/methods

1. Deep learning: Neural Networks (NN), Convolutional NN, Recurrent NN, Boltzmann machines, autoencoders and variational autoencoders and generative adversarial networks, stable diffusion and many more generative models
2. Bayesian statistics and Bayesian Machine Learning, Bayesian experimental design, Bayesian Regression models, Bayesian neural networks, Gaussian processes and much more
3. Dimensionality reduction (Principal component analysis), Clustering Methods and more
4. Ensemble Methods, Random forests, bagging and voting methods, gradient boosting approaches
5. Linear and logistic regression, Kernel methods, support vector machines and more
6. Reinforcement Learning; Transfer Learning and more

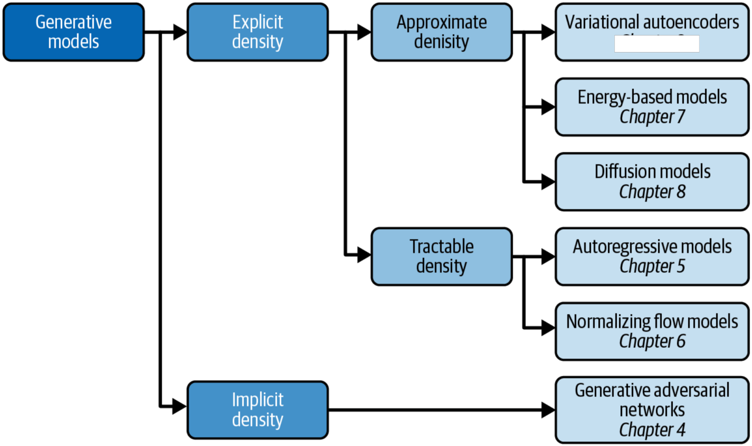
Example of discriminative modeling, taken from Generative Deep Learning by David Foster



Example of generative modeling, taken from Generative Deep Learning by David Foster



Taxonomy of generative deep learning, taken from Generative Deep Learning by David Foster



Good books with hands-on material and codes

- Sebastian Rashcka et al, Machine learning with Sickit-Learn and PyTorch
- David Foster, Generative Deep Learning with TensorFlow
- Babcock and Gavras, Generative AI with Python and TensorFlow 2

All three books have GitHub sites from where one can download all codes. A good and more general text (2016) is Goodfellow, Bengio and Courville, Deep Learning

More references

Reading on diffusion models

1. A central paper is the one by Sohl-Dickstein et al, Deep Unsupervised Learning using Nonequilibrium Thermodynamics, https://arxiv.org/abs/1503.03585
2. See also Diederik P. Kingma, Tim Salimans, Ben Poole, Jonathan Ho, Variational Diffusion Models, https://arxiv.org/abs/2107.00630

and VAEs

1. An Introduction to Variational Autoencoders, by Kingma and Welling, see https://arxiv.org/abs/1906.02691

And two Nobel prizes this year. Physics and Chemistry

What are the basic Machine Learning ingredients?

Almost every problem in ML and data science starts with the same ingredients:

- The dataset $\boldsymbol{x}$ (could be some observable quantity of the system we are studying)
- A model which is a function of a set of parameters $\boldsymbol{\alpha}$ that relates to the dataset, say a likelihood function $p(\boldsymbol{x}|\boldsymbol{\alpha})$ or just a simple model $f(\boldsymbol{\alpha})$
- A so-called **loss/cost/risk** function $\mathcal{C}(\boldsymbol{x}, f(\boldsymbol{\alpha}))$ which allows us to decide how well our model represents the dataset.

We seek to minimize the function $\mathcal{C}(\boldsymbol{x}, f(\boldsymbol{\alpha}))$ by finding the parameter values which minimize $\mathcal{C}$. This leads to various minimization algorithms. It may surprise many, but at the heart of all machine learning algortihms there is an optimization problem.

Low-level machine learning, the family of ordinary least squares methods

Our data which we want to apply a machine learning method on, consist of a set of inputs $\boldsymbol{x}^T = [x_0, x_1, x_2, \dots, x_{n-1}]$ and the outputs we want to model $\boldsymbol{y}^T = [y_0, y_1, y_2, \dots, y_{n-1}]$. We assume that the output data can be represented (for a regression case) by a continuous function f through

$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon.$$

Setting up the equations

In linear regression we approximate the unknown function with another continuous function $\tilde{\boldsymbol{y}}(\boldsymbol{x})$ which depends linearly on some unknown parameters $\boldsymbol{\theta}^T = [\theta_0, \theta_1, \theta_2, \dots, \theta_{p-1}]$.
The input data can be organized in terms of a so-called design matrix with an approximating function $\tilde{\boldsymbol{y}}$

$$\tilde{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{\theta},$$

The objective/cost/loss function

The simplest approach is the mean squared error

$$C(\boldsymbol{\Theta})=\frac{1}{n}\sum_{i=0}^{n-1}\left(y_i-\tilde{y}_i\right)^2=\frac{1}{n}\left\{\left(\boldsymbol{y}-\boldsymbol{\tilde{y}}\right)^T\left(\boldsymbol{y}-\boldsymbol{\tilde{y}}\right)\right\},$$

or using the matrix $\boldsymbol{X}$ and in a more compact matrix-vector notation as

$$C(\boldsymbol{\Theta})=\frac{1}{n}\left\{\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\theta}\right)^T\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\theta}\right)\right\}.$$

This function represents one of many possible ways to define the so-called cost function.

Training solution

Optimizing with respect to the unknown parameters θ_j we get

$$\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\theta},$$

and if the matrix $\boldsymbol{X}^T\boldsymbol{X}$ is invertible we have the optimal values

$$\hat{\boldsymbol{\theta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

We say we 'learn' the unknown parameters $\boldsymbol{\theta}$ from the last equation.

Selected references

- Mehta et al. and Physics Reports (2019).
- Machine Learning and the Physical Sciences by Carleo et al
- Artificial Intelligence and Machine Learning in Nuclear Physics, Amber Boehnlein et al., Reviews Modern of Physics 94, 031003 (2022)
- Particle Data Group summary on ML methods

Scientific Machine Learning

An important and emerging field is what has been dubbed as scientific ML, see the article by Deiana et al, Applications and Techniques for Fast Machine Learning in Science, Big Data **5**, 787421 (2022) https://doi.org/10.3389/fdata.2022.787421

The authors discuss applications and techniques for fast machine learning (ML) in science – the concept of integrating power ML methods into the real-time experimental data processing loop to accelerate scientific discovery. The report covers three main areas

1. applications for fast ML across a number of scientific domains;
2. techniques for training and implementing performant and resource-efficient ML algorithms;
3. and computing architectures, platforms, and technologies for deploying these algorithms.

ML for detectors

ELSEVIER

Engineering

Volume 6, Issue 3, March 2020, Pages 264-274

Research Artificial Intelligence—Review

A Survey of Accelerator Architectures for Deep Neural Networks

Yiran Chen [a], Yuan Xie [b], Linghao Song [a], Fan Chen [a], Tianqi Tang [b]

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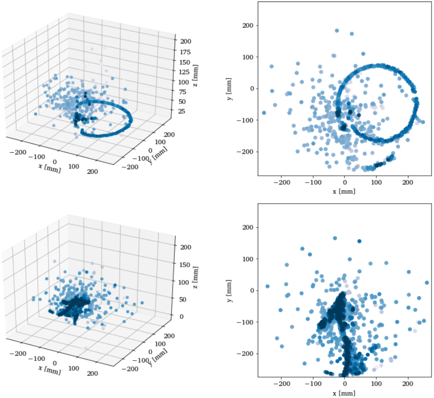
https://doi.org/10.1016/j.eng.2020.01.007

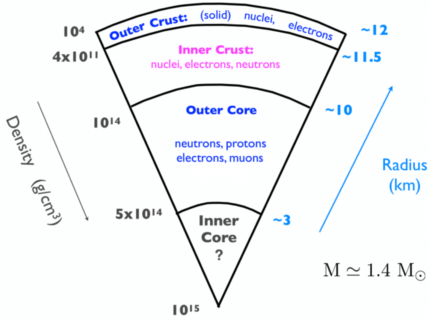
Abstract

Argon-46 by Solli et al., NIMA 1010, 165461 (2021)

Representations of two events from the Argon-46 experiment. Each row is one event in two projections, where the color intensity of each point indicates higher charge values recorded by the detector. The bottom row illustrates a carbon event with a large fraction of noise, while the top row shows a proton event almost free of noise.

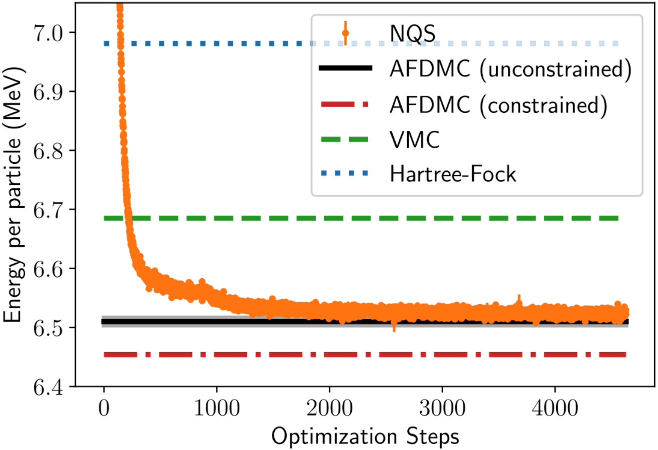


Neutron star structure



- Mostly neutrons but composition varies with density
- Nuclei in crust are squeezed into uniform matter in core
- Likely neutron superfluid in inner crust and outer core
- Calculations currently focus on inner crust

Dilute neutron star matter from neural-network quantum states by Fore et al, Physical Review Research 5, 033062 (2023) at density $\rho = 0.04\ \mathrm{fm}^{-3}$



Education and advanced training

1. Outreach and communication on quantum technologies and AI, explaining quantum technologies and AI to a broader audience
2. Research on education in AI and QT. How are these topics best communicated and implemented in different enviroments, from high school education to universities and to a broader audience, including external partners
3. QAI-TALENT, Education and knowledge transfer through the development of advanced educational programs

Education, Quantum and AI/Machine Learning

At the university of Oslo we have now established several educational programs in AI and QTs and quantum science. These programs span the whole spectrum from beginners courses to advanced training and education tailored to the specific needs of the participants.
Furthermore, through research done at the center for Computing in Science Education and the physics education research group at the department of physics of the university of Oslo, we have over the years developed knowledge and insights on how to teach central concepts in quantum science as well as developing computational literacy and understanding of central algorithms applied to scientific problems.

Courses and study programs

1. **New study direction on Quantum technology** in Bachelor program Physics and Astronomy, starts Fall 2024. Three new courses:
   - FYS1400 Introduction to Quantum Technologies
   - FYS3405/4405 Quantum Materials
   - FYS3415/4415 Quantum Computing
2. **Developed Master of Science program on Computational Science**, started fall 2018 and many students here work on quantum computing and machine learning
3. Developed courses on machine learning, from basic to advanced ones
4. Developed advanced course on quantum computing and quantum machine learning, MAT3420, MAT4430/9430, FYS5419/9419
5. New study directions in Master of Science in Physics and Computational Science on Quantum technologies and more. Start fall 2025

Content of courses we offer

1. Quantum Information theory
2. From Classical Information theory to Quantum Information theory
3. Classical and Quantum Laboratory
4. Discipline-Based Quantum Mechanics
5. Quantum algorithms, computing, software and hardware
6. Several machine learning/AI courses, at all levels

QAI-TALENT: Education for a broader audience

We have yearslong experience (with research based evidence on what works or not) in developing intensive training courses on ML/AI and QT. We plan to develop an educational activity on quantum science and AI, **QAI TALENT** (TALENT=Training and Advanced Lectures in EmergiNg Technologies) offering

1. Intensive short courses on selected topics (which can lead to credits and certificates)
2. Certificates of expertise with modules that can add up to one year of credits or more.
3. Possibilities of adding up to a master specialization in quantum science/technologies and/or AI/ML
4. Common educational projects and supervision of students

1st and 2nd quantum revolution

Overview of quantum technologies

Status and opportunities

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1st and 2nd quantum revolution

Overview of quantum technologies

Status and opportunities

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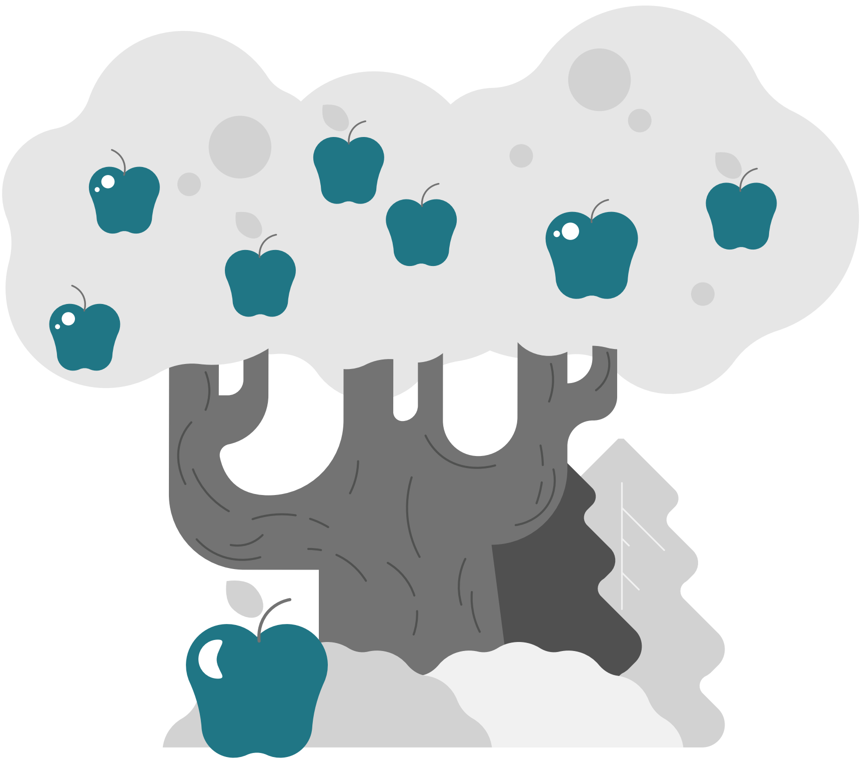
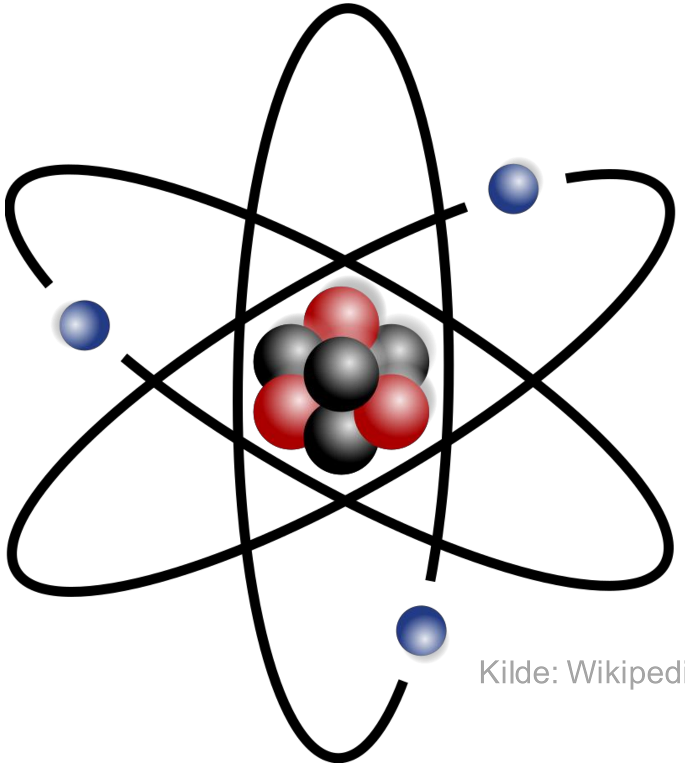
From classical to quantum physics





Kilde: Wikipedia

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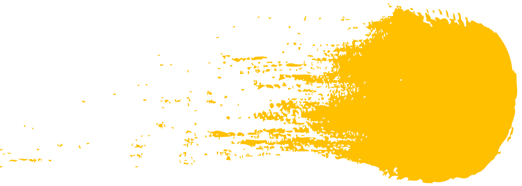
The 1st quantum revolution: Quantum physics experiments

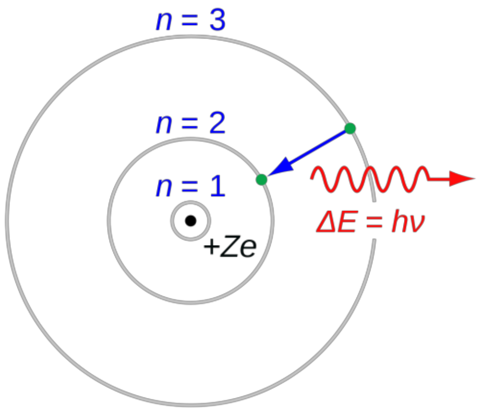
Max Planck, Albert Einstein, Arthur Compton



Light can behave like particles

Photons have momentum

Niels Bohr



Quantum systems have discrete (quantized) energy levels

Louis de Broglie

Particle-wave duality

Particles can exhibit wave-like properties

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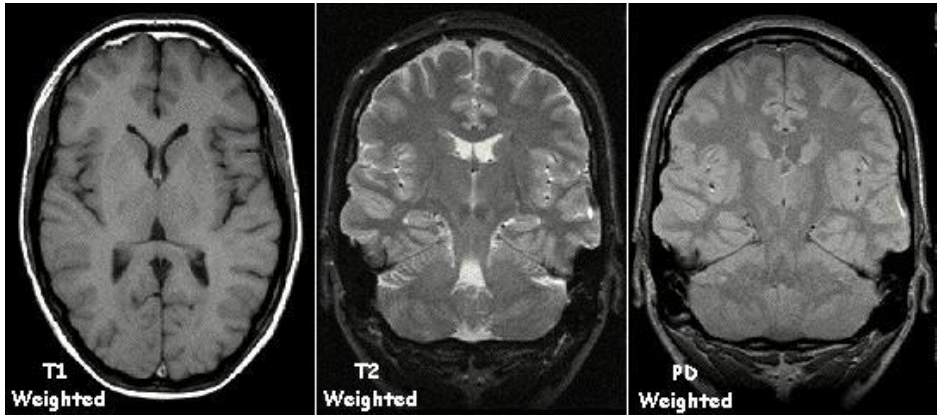
Quantum revolution 1.5: Macroscopic quantum properties



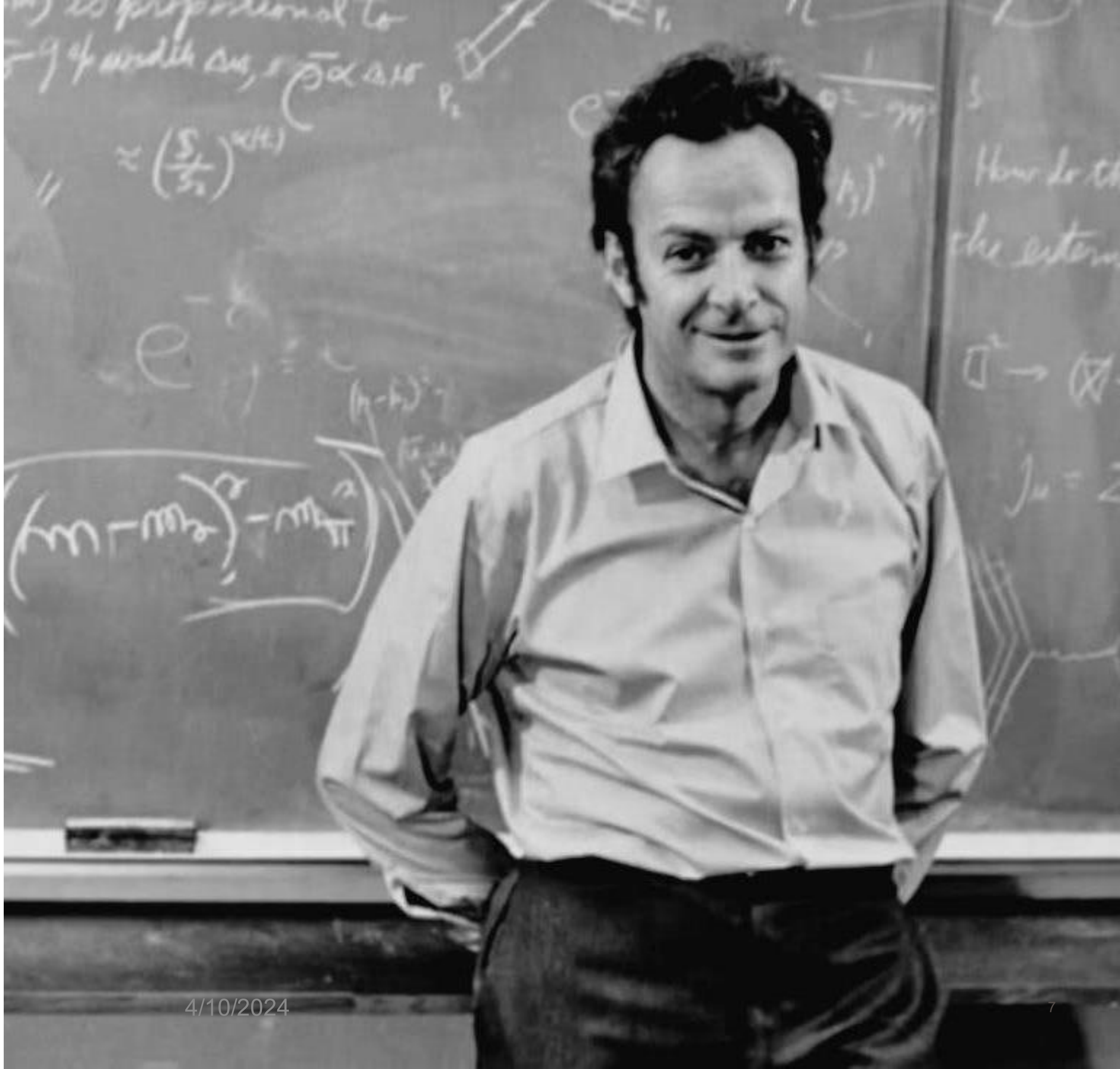
https://en.wikipedia.org/wiki/Magnetoresistive_RAM#/media/File:200mm_1_Mb_MRAM_-_D60_Symposium_-_Defense_Advanced_Research_Projects_Agency_-_DSC05568.jpg
By KieranMaher at English Wikibooks https://commons.wikimedia.org/w/index.php?curid=12766438
https://commons.wikimedia.org/wiki/File:RBG-LED.jpg

“nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical.”

Richard Feynman

Quantum technology exploits the unique and exotic properties of quantum mechanics

- Superposition
- Quantum entanglement
- Tunneling



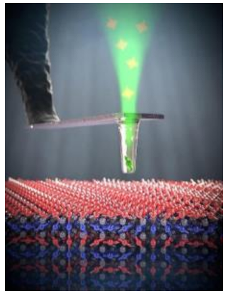
The 2nd quantum revolution: Direct control over quantum systems

1. Computing	2. Sensing	3. Communication
• Information processing • Solve tasks not possible with classical computing	• Nanoscale spatial resolution • Fast response	• Transmit information • Quantum security

Quantum technology promises new opportunities

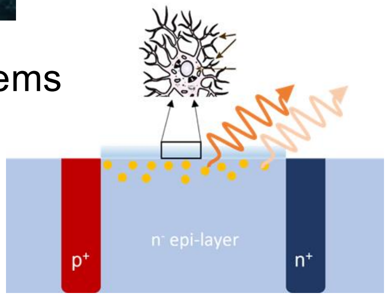
Extreme conditions

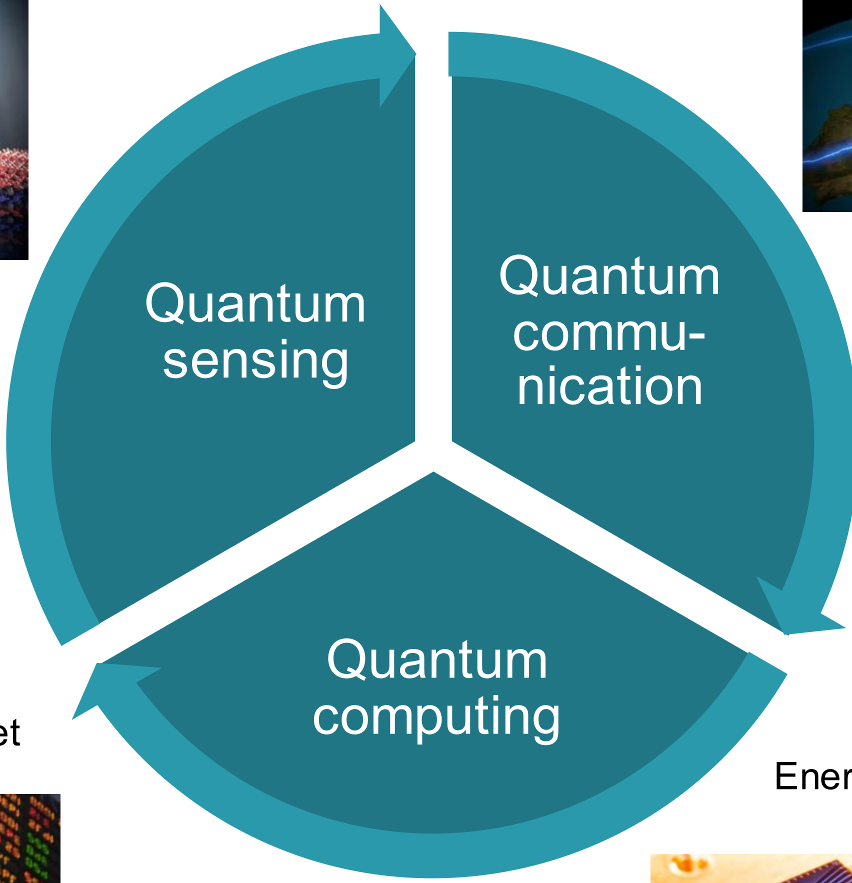
Nanoscale



Better control systems

Signals in cells





Quantum internet

Quantum cryptography

Secure communication based on laws of quantum physics

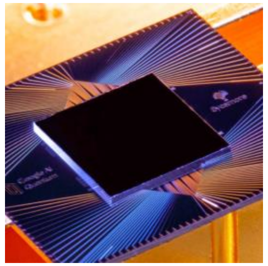
Model finance market

Model weather, climate

Better logistics

Optimized energy consumption

Energy efficient computation



Find new drugs and materials for green transition

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1st and 2nd quantum revolution

Overview of quantum technologies

Status and opportunities

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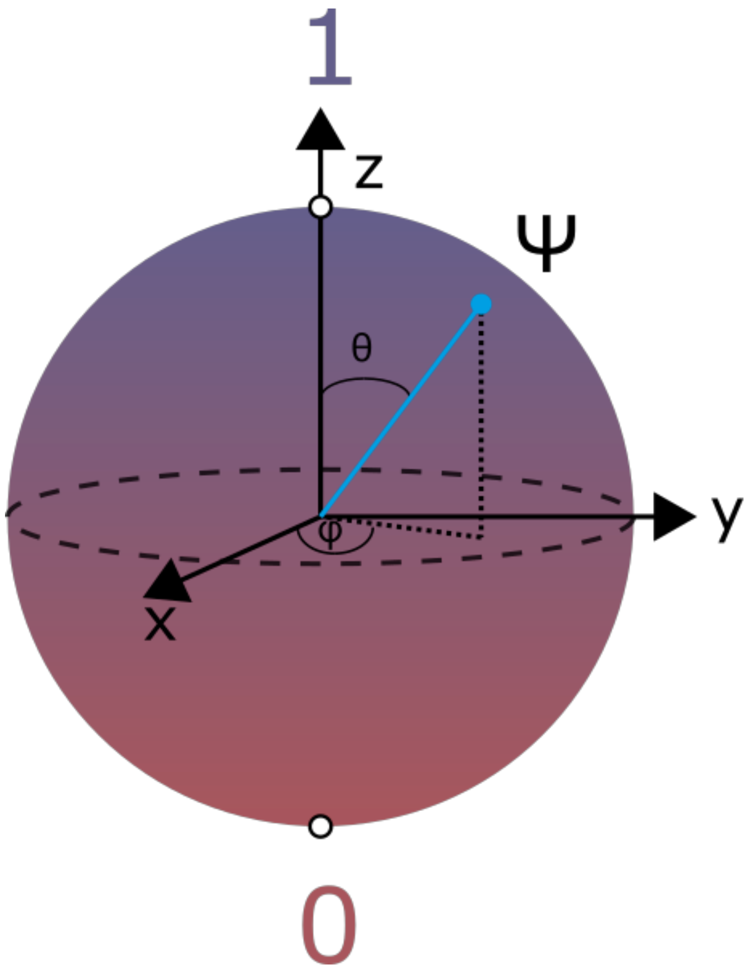
Quantum bits: the building block of quantum technology

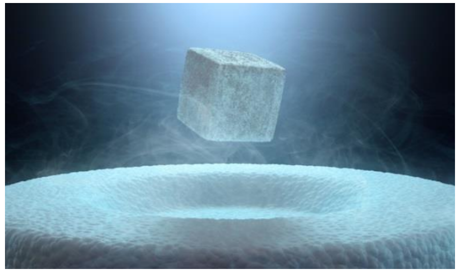
Qubit guidelines:

1. Stable, two-level quantum system
2. Communication path
3. Scalable
4. Energy efficient



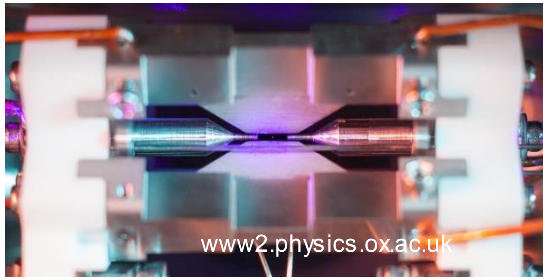
Choice of material platform depends on application

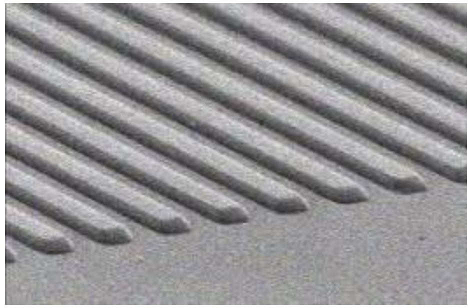
- Superconductors
- Trapped ions
- Optical gratings
- Quantum dots
- Defects in semiconductors
- …



Superconductors

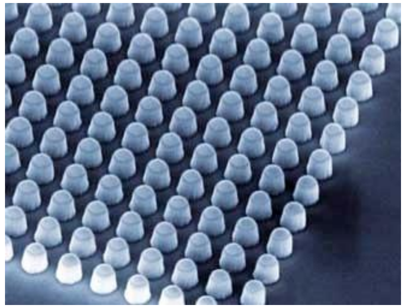
Trapped ions

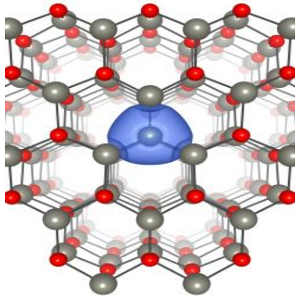




Optical gratings

Quantum dots





Semiconductor
point defects

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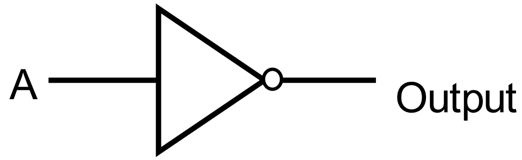
1. Gate model for quantum computing

Logic gates

- Classical circuits based on logic gates
- Gates perform logic operations
  - Rules for answering YES/NO questions
  - Input is 1 and 0 from transistors/bits

Example: NOT (inverter)

A	Output
0	1
1	0



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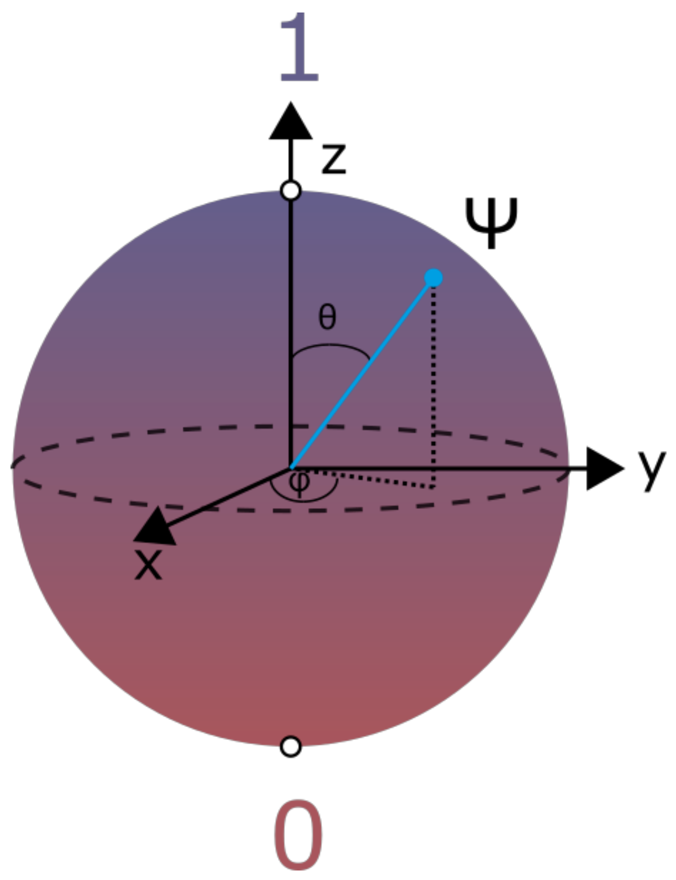
Quantum logic gates

- Most popular architecture for QC
- Inspired by classical logic gates
- Manipulate qubits by gate operations
- Quantum circuits are formed by qubits and quantum gates

Quantum gate operations

- Quantum gates can operate on one, two or more qubits
- We represent quantum gates by unitary matrices (U*U=I)
  - 1-qubit gates are 2×2 matrices
  - 2-qubit gates have 16 matrix elements, etc.
- In practice; e.g. pulse of electromagnetic field

Represent qubits as a vector along a Bloch-sphere



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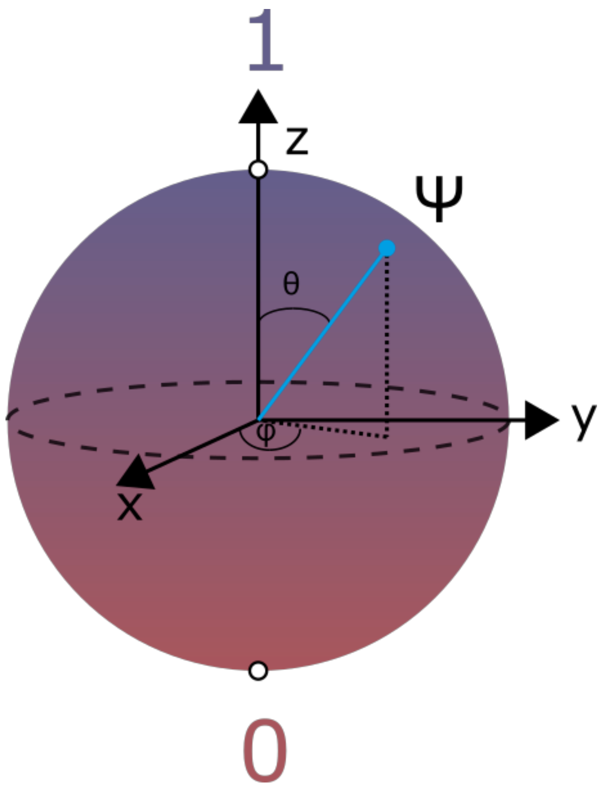
One-qubit quantum gates

X gate

- Quantum NOT
- Performs bit flip (0-to-1 and 1-to-0)

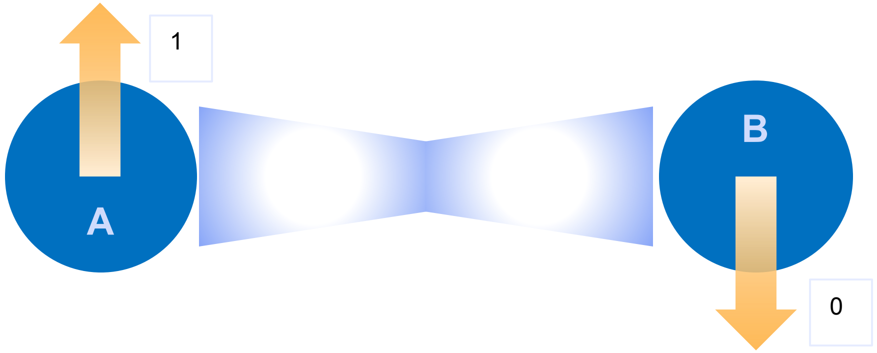
Hadamard gate

- Quantum analog to one-qubit Fourier transform
- Transforms a basis state (0 or 1) to a superposition of states



Controlled NOT (CNOT)

CNOT can generate a maximally entangled state between two qubits

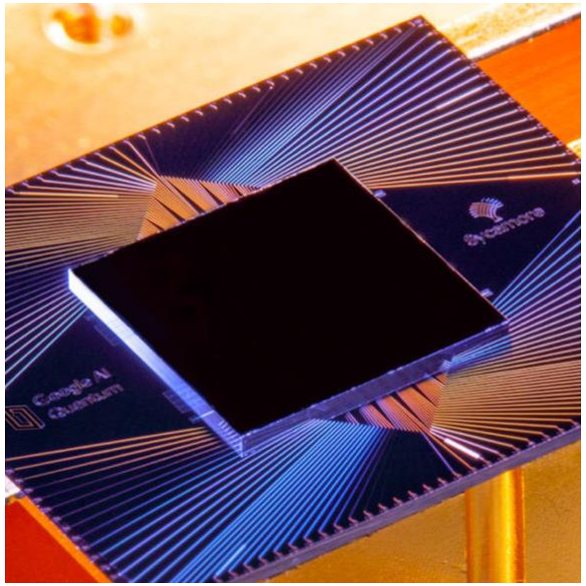


Satus for quantum computing

Where are we now?

- Noisy intermediate-scale quantum (NISQ)
- Superconducting qubits
- Quantum advantage is debatable

- Ideal time to learn!



https://www.nature.com/articles/s41586-019-1666-5

https://www.ibm.com/quantum/roadmap

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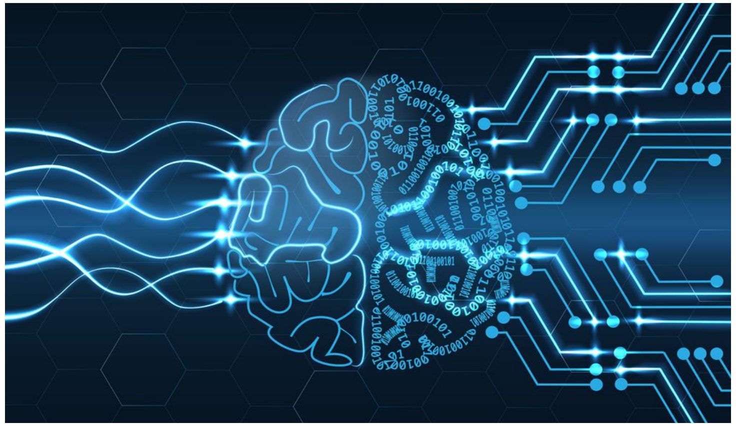
2. Sensors are the foundation of the digital and green shifts

Kilde: Wikipedia

Better control systems

Improved safety



Input to AI

https://iot.eetimes.com/the-power-and-potential-of-applying-artificial-intelligence-to-sensor-generated-data/

Optimized energy consumption

Need for quantum sensors

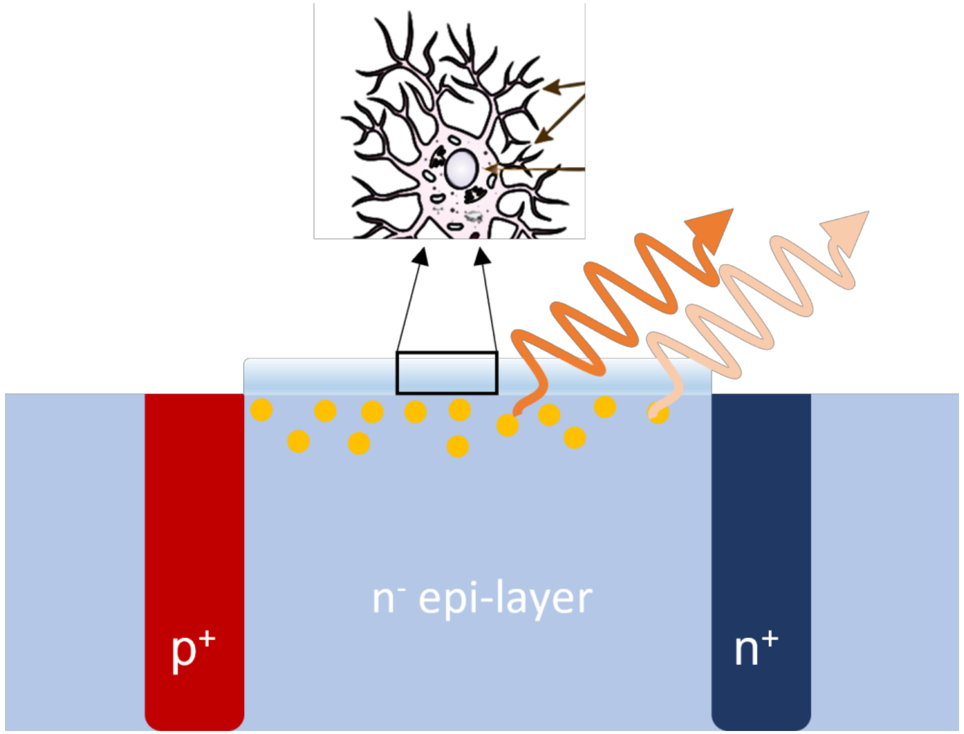
Limitations of today's technology

- Limitation in detection
  - Spatial resolution
  - Sensitivity
  - Extreme conditions

- Limitation in operation
  - Speed
  - Extreme conditions

Next generation: Quantum sensors

- Nanoscale spatial resolution, fast detection and extreme conditions possible
- Sensitivity beyond classical limit



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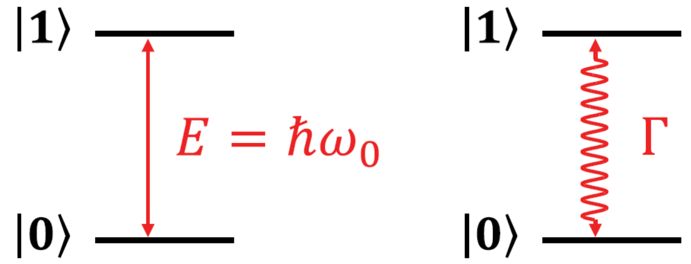
What is quantum sensing ?

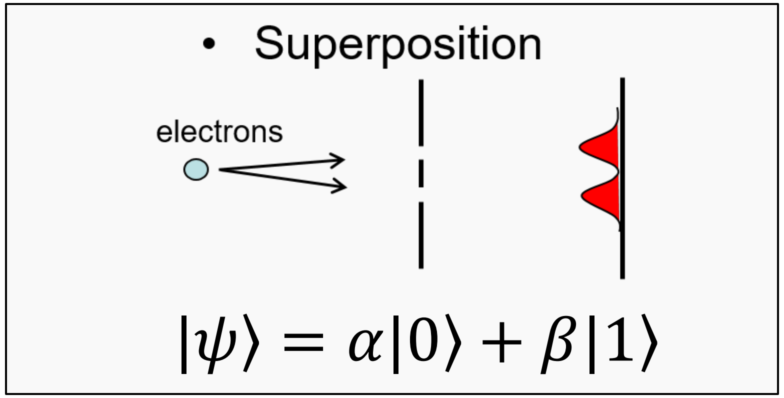
Definitions:

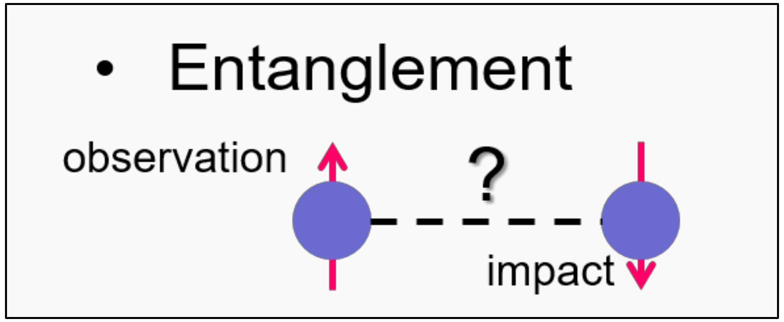
1. Use of quantum system with quantized energy levels to measure a physical quantity

2. Use of quantum coherence (i.e., wavelike spatial or temporal superposition states) to measure a physical quantity.

3. Use of quantum entanglement to improve the sensitivity or precision of a measurement, beyond what is possible classically



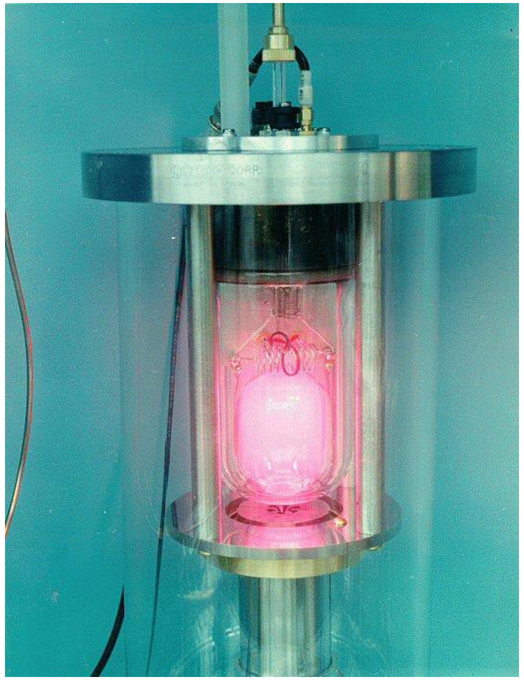




Degen et al., Rev. Mod. Phys., Vol. 89, No. 3, (2017)

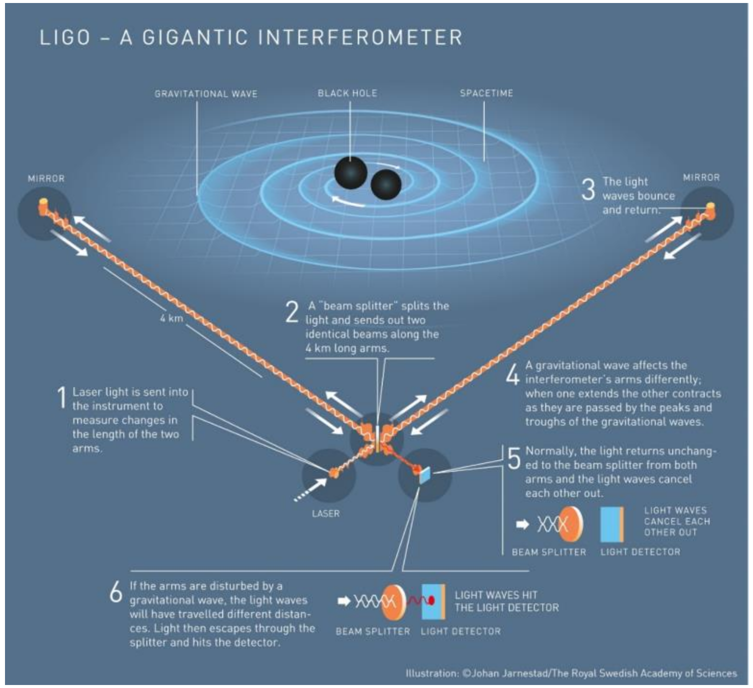
Early examples of quantum sensors

Atomic clock

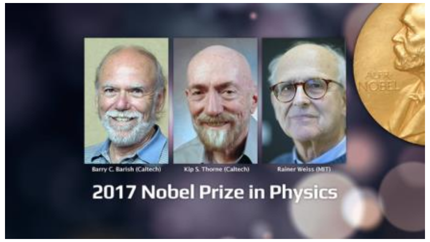


Kilde: Wikipedia

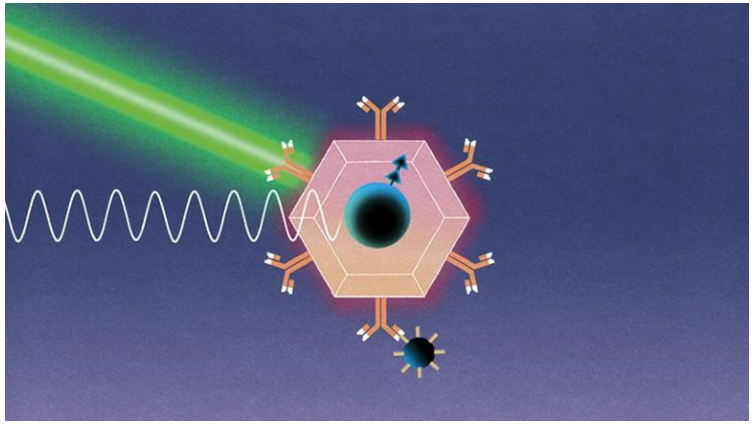
LIGO: Gravitational wafer



LIGO collab., Nature Photonics, 7, 613 (2013)



NV-centres in diamond (semiconductor-based) for biological sensing



Nature 591, S37 (2021)

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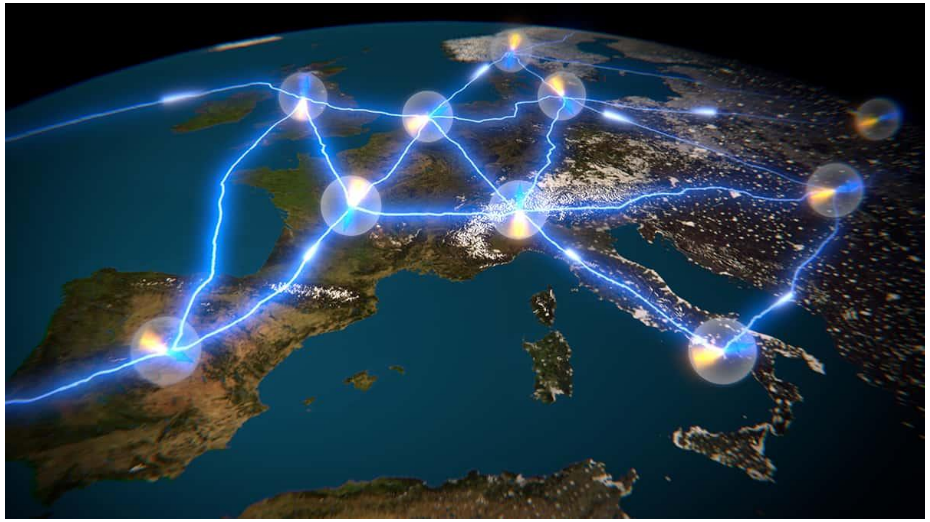
3. Quantum communication

Transferring a quantum state from one place to another

Application areas

- Provably secure communication
- Quantum networks
  - o Optical fiber network
  - o Free space network
  - o Part of quantum computers
- Secure quantum internet



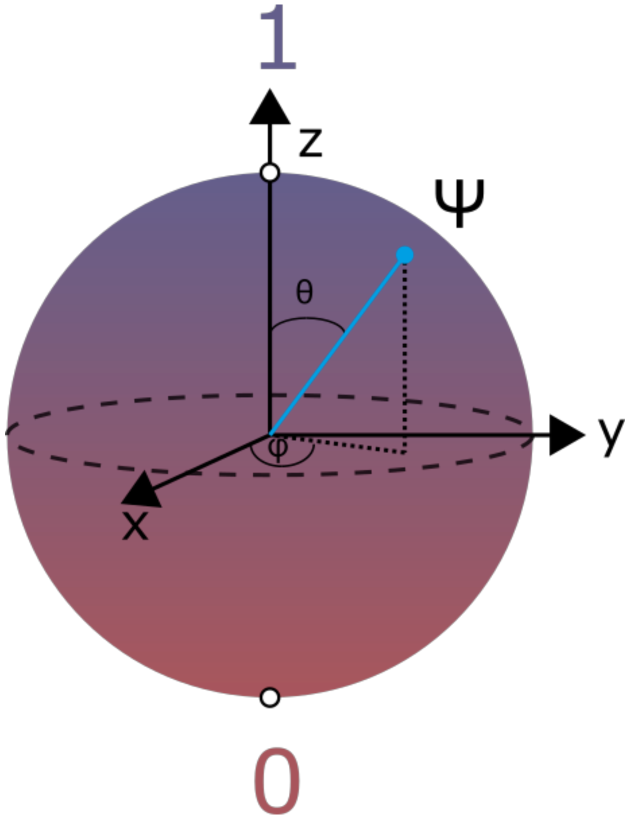
https://www.wired.com/sponsored/story/with-quantum-computings-rise-cybersecurity-takes-center-stage/
https://physicsworld.com/a/a-roadmap-for-the-quantum-internet/

Transmitting information
Flying qubits

Individual or entangled photons are used to transmit data in a provably secure way

Degree of freedom to encode information in

- Spatially encoded qubits
- Temporal structure
- **State of polarization**



Advantage of photonic polarization qubits

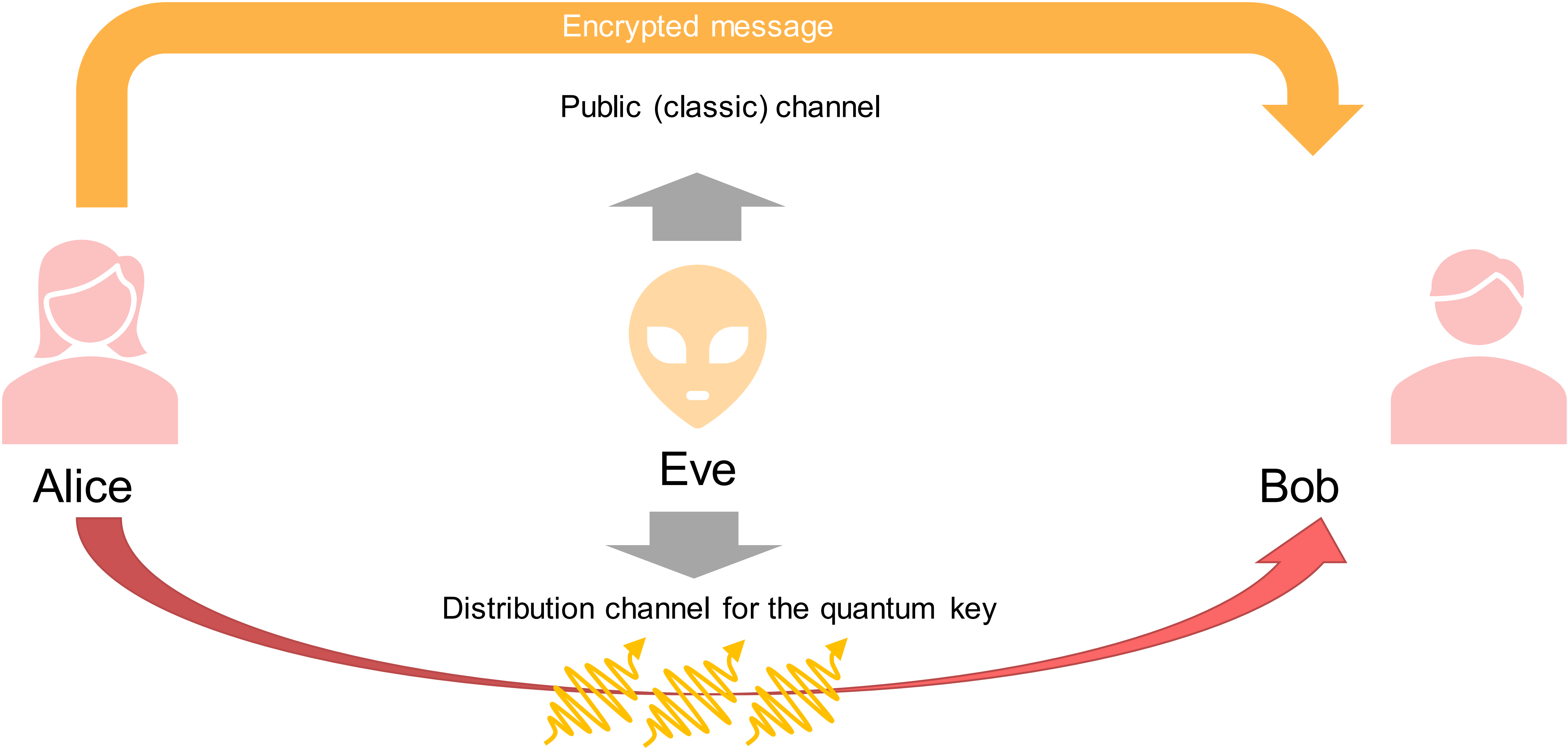
- Easily generated and manipulated
- Photons interact little with the environment

Why quantum communication?
Security in the quantum age

https://www.healthcarecompliancepros.com/blog/usa-leads-the-way-with-the-most-expensive-healthcare-data-breaches

IBM Research, https://www.flickr.com/photos/ibm_research_zurich/51248690716/, CC BY 2.0

Security through quantum mechanics
Quantum key distribution (QKD)



1st and 2nd quantum revolution

Overview of quantum technologies

Status and opportunities

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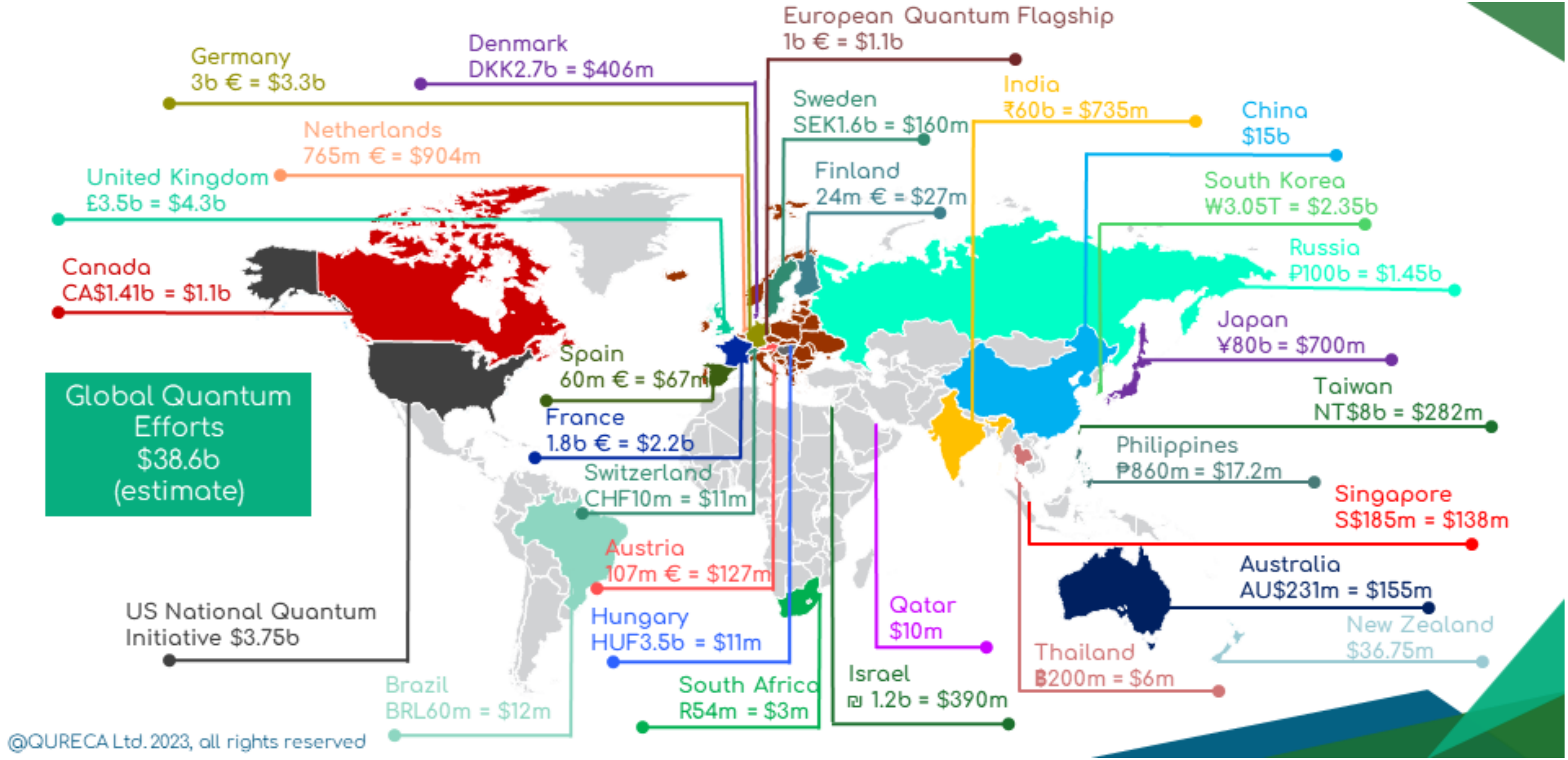
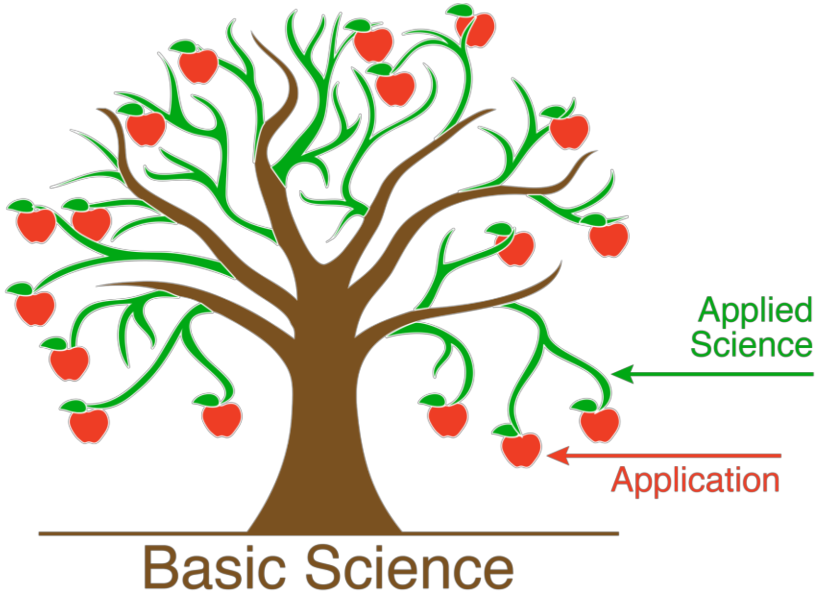
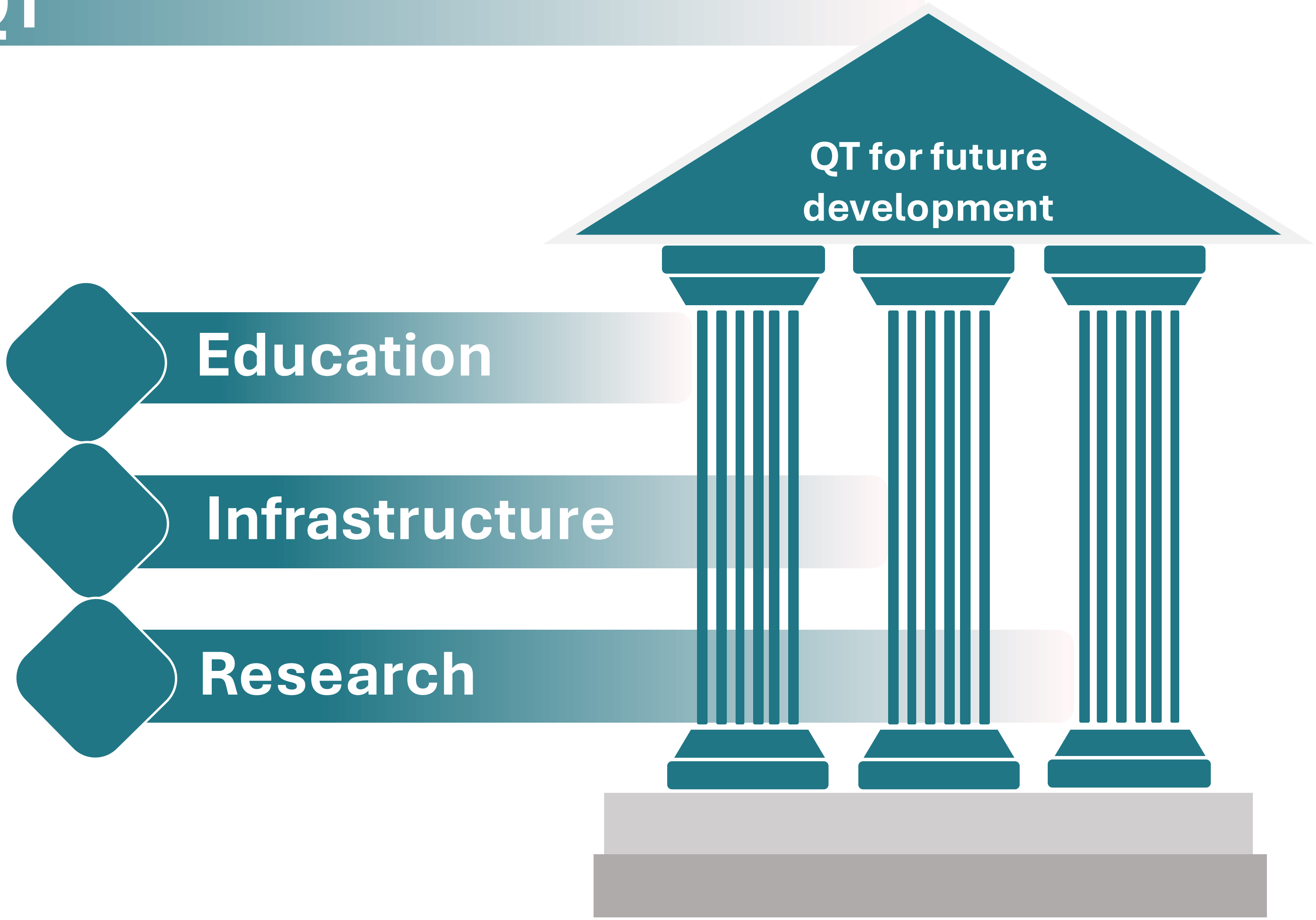
Quantum technology is a major theme in research and technology development



UiO is investnig in QT

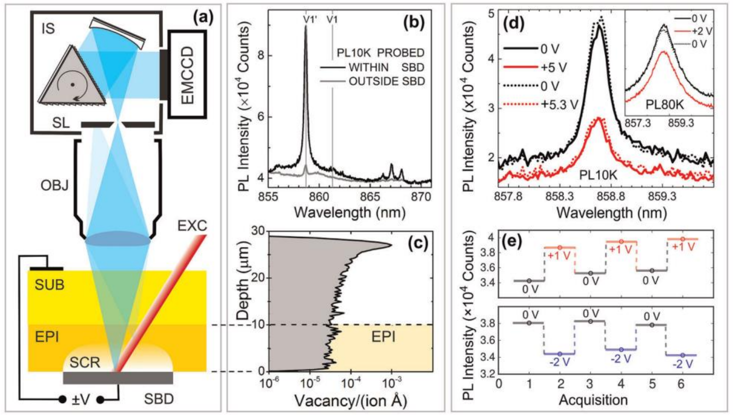




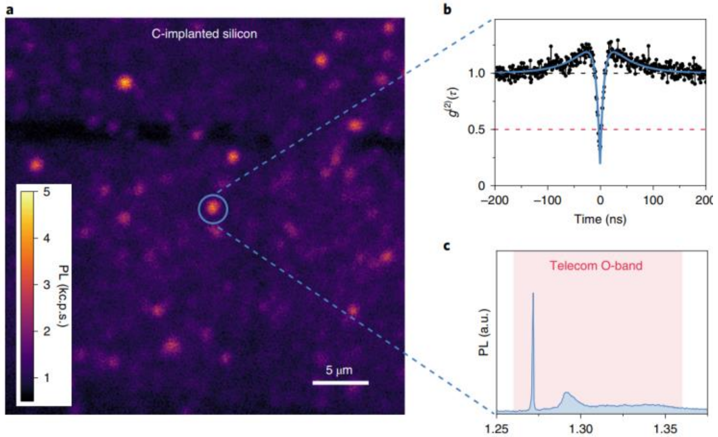
Research

- UiO has extensive theoretical, computational and experimental quantum science and technology
- Semiconductors for sustainable QT
- Quantum sensors will be strategically important for Norway

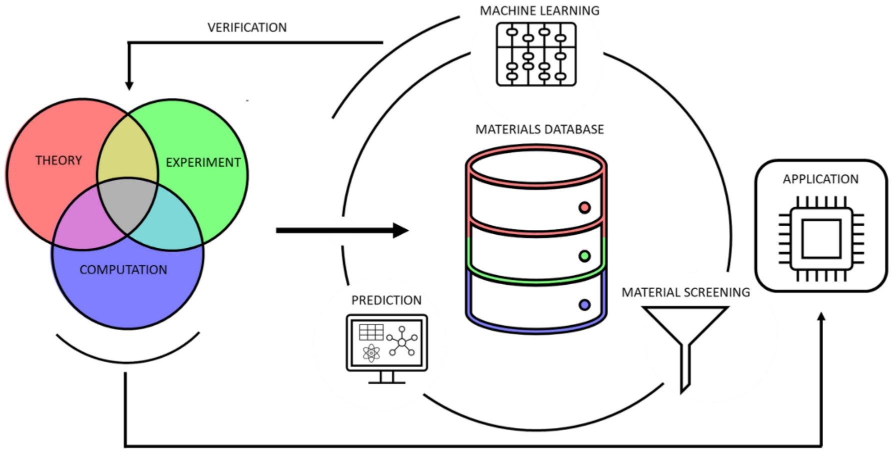
Collaboration between research, start-ups, industry and public sector is needed



npj Quantum Information, vol. 5, 111 (2019).



Nature Electronics, vol. 3, 738 (2020).



npj Comp Mat, vol. 8, 207 (2022).

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