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Welcome

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The Quantum Women Invited Talk Series

Presenter: Philippa Rubin

March 29th 2023

Presenter introduction

My name is Philippa Rubin

I am a Research Software Engineer at the Science and Technology Facilities Council (STFC)

STFC supports research in astronomy, physics and space science, and operates world-class research facilities for the UK

Background in mathematics, spend the majority of my time working on quantum computing projects at the Hartree Centre

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My background

I am where I am today because I have always loved maths!

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Studied Mathematics at Imperial College London

Graduated 2019

UKRI
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Hartree Centre

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-zsh
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→ . .venv/bin/activate

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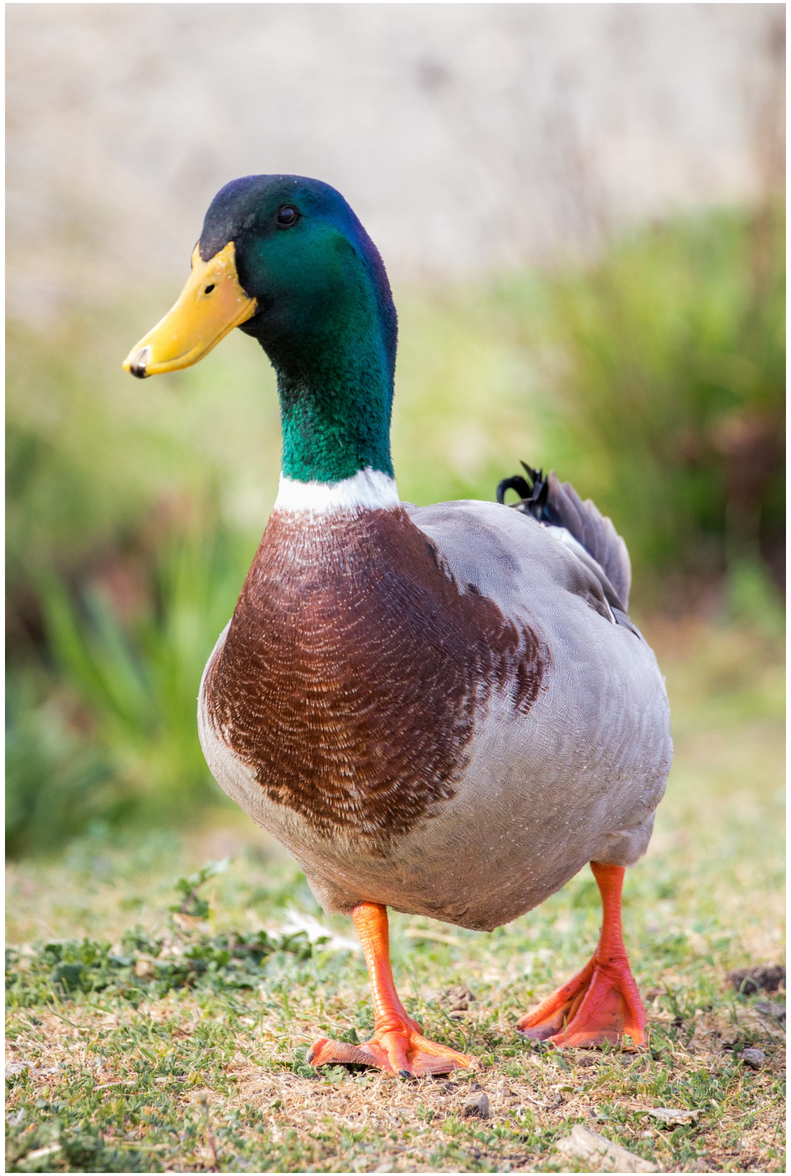

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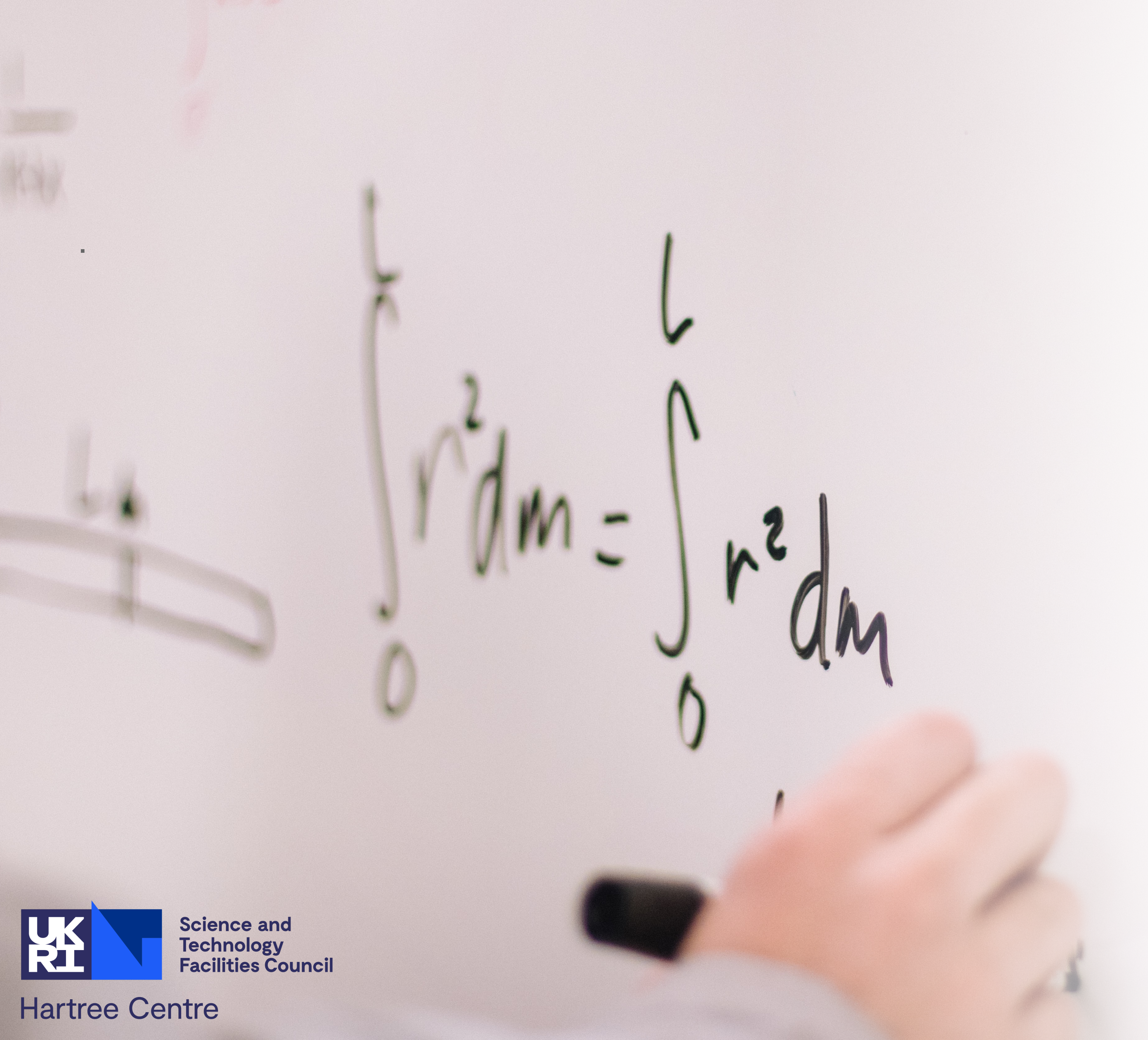

- Lots of options when you go to university, often have a catalogue of courses to pick from in your chosen subject
- I wasn't too picky – I liked everything
- I did lots of pure maths courses, which includes things like analysis, algebra… and applied maths courses, such as statistics, computing, physics

But I liked studying quantum mechanics because it brought lots of different areas of mathematics together

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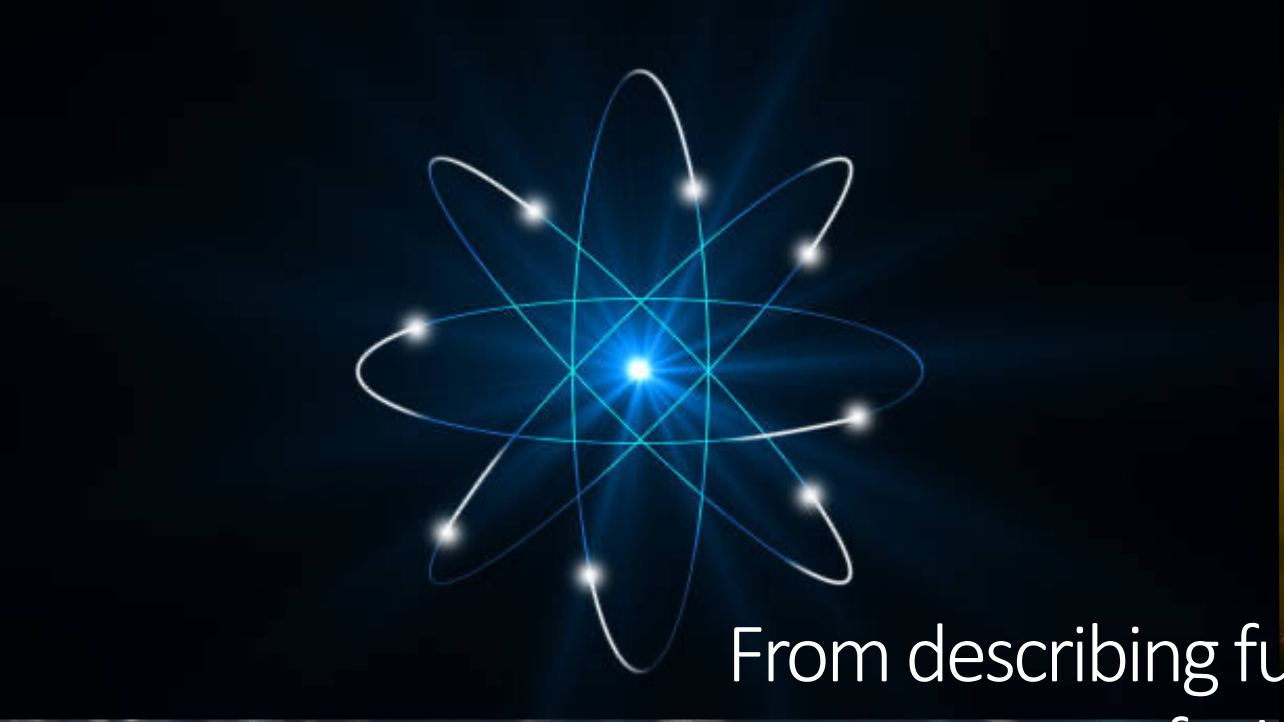
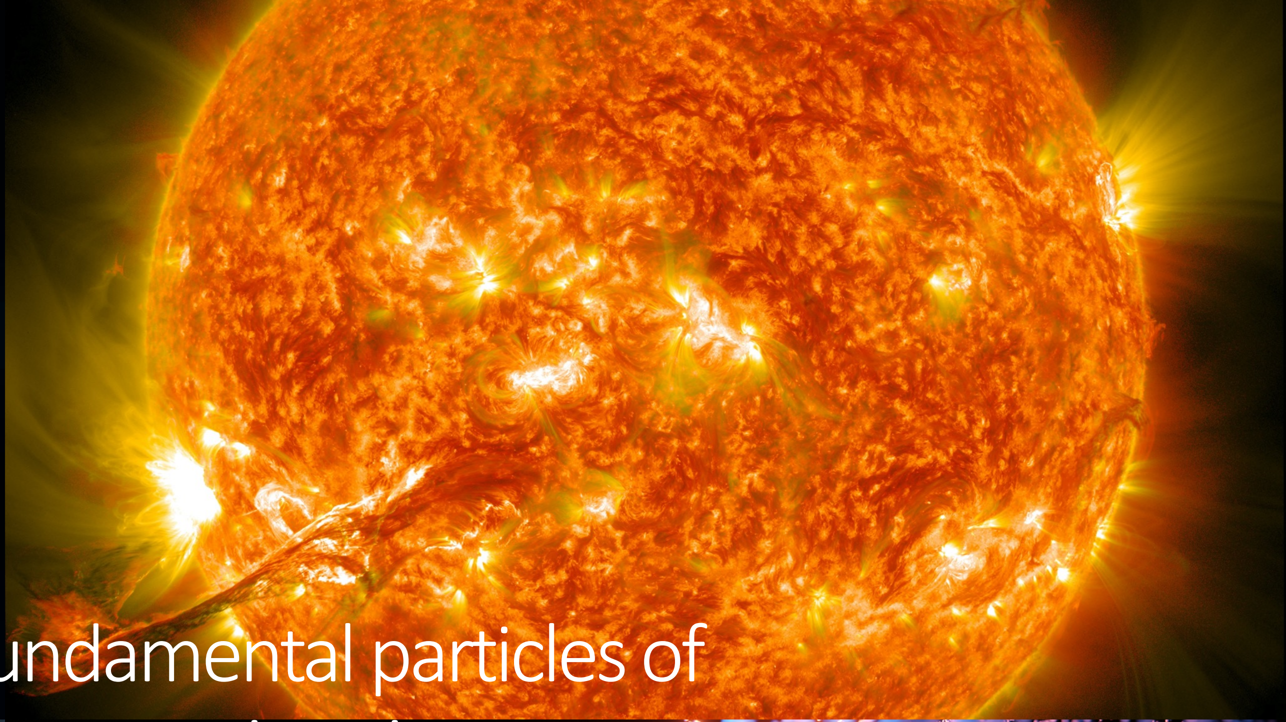
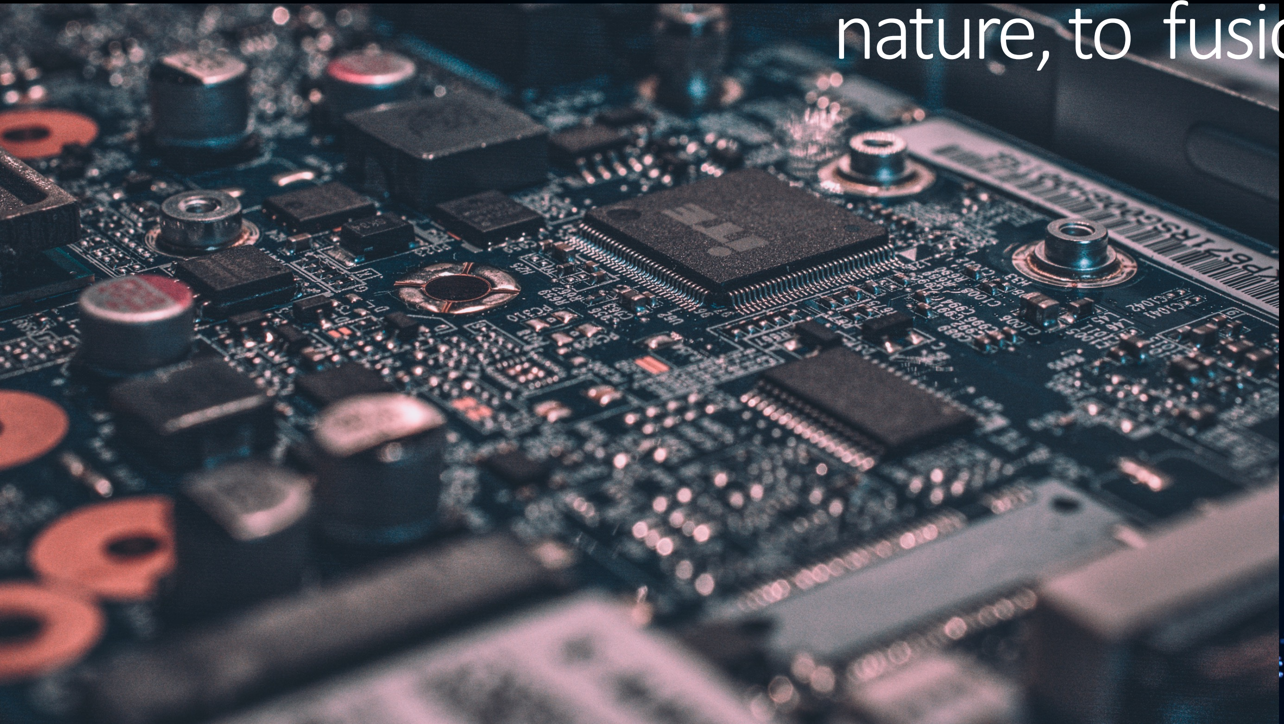
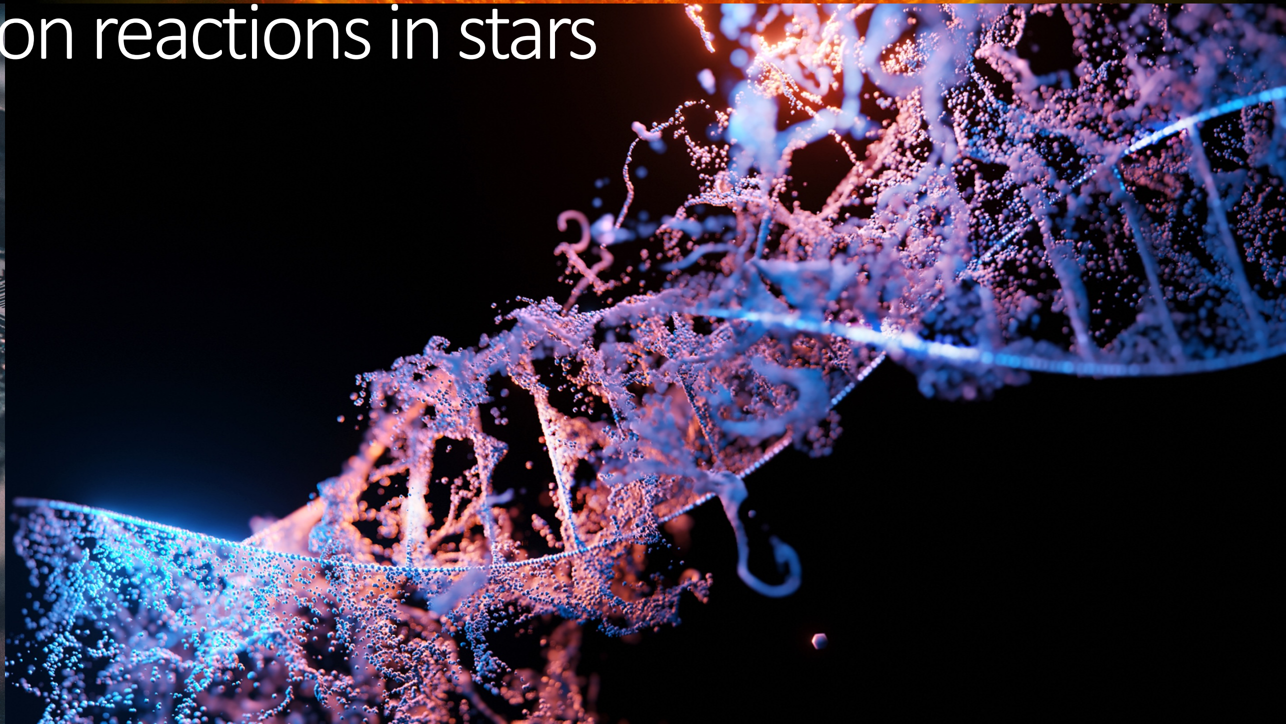
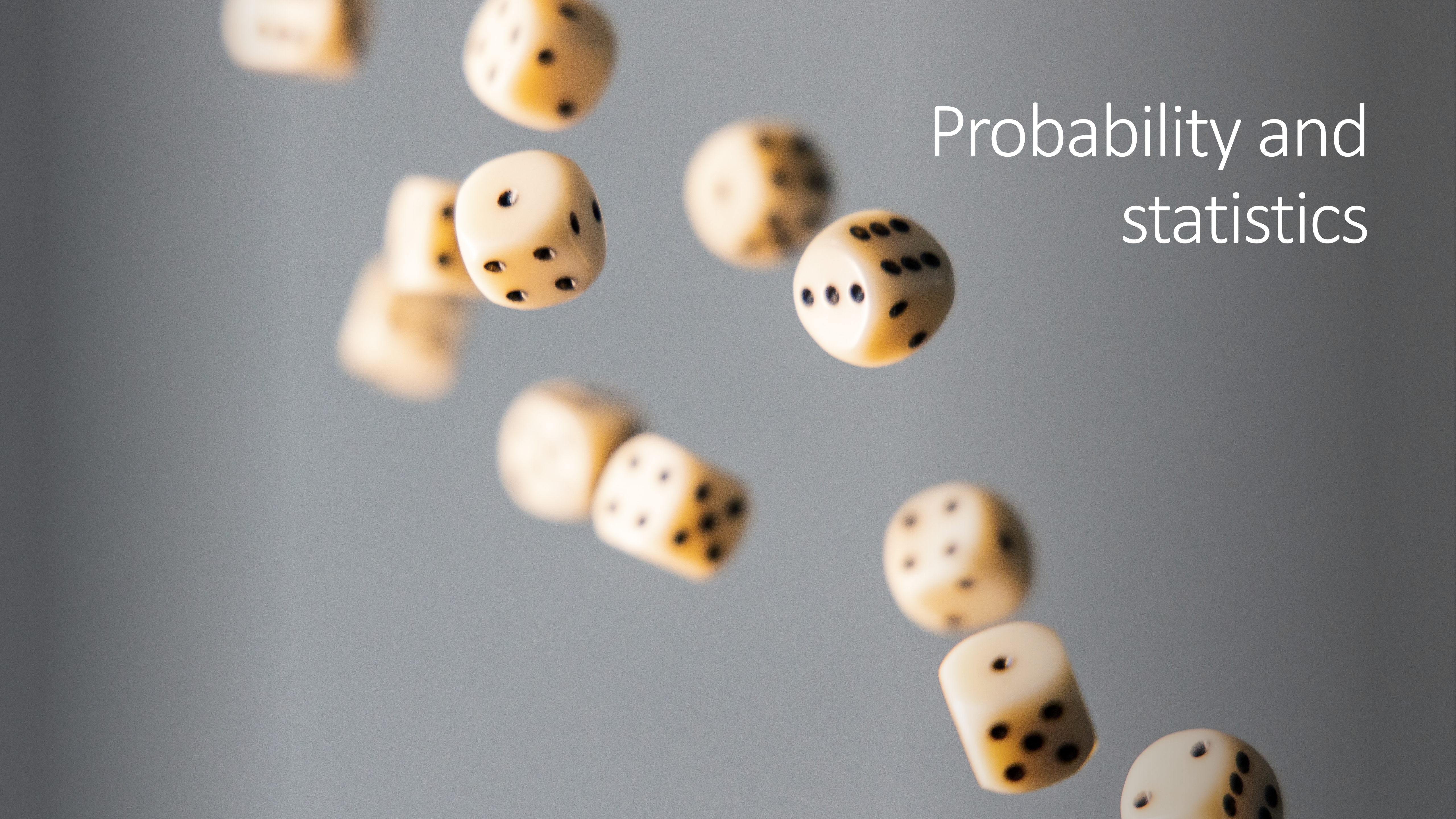
Describing how the universe works

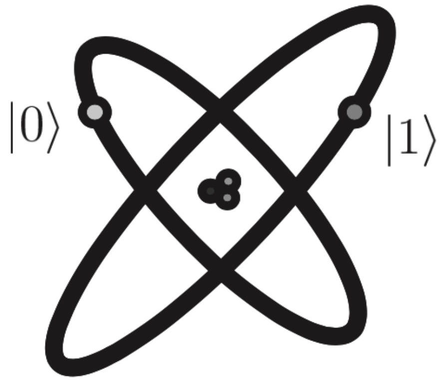



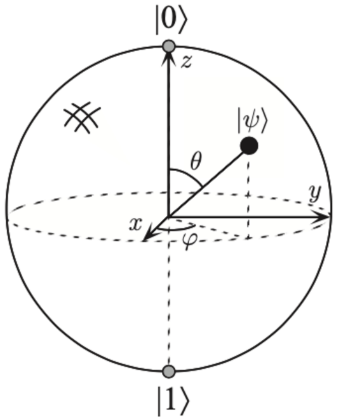
From describing fundamental particles of nature, to fusion reactions in stars

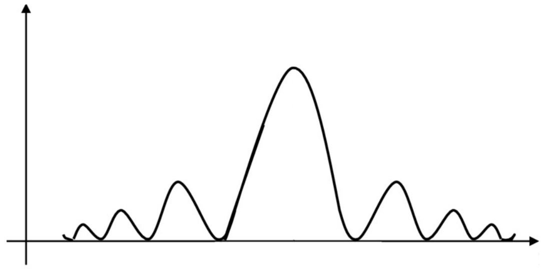



Probability and statistics



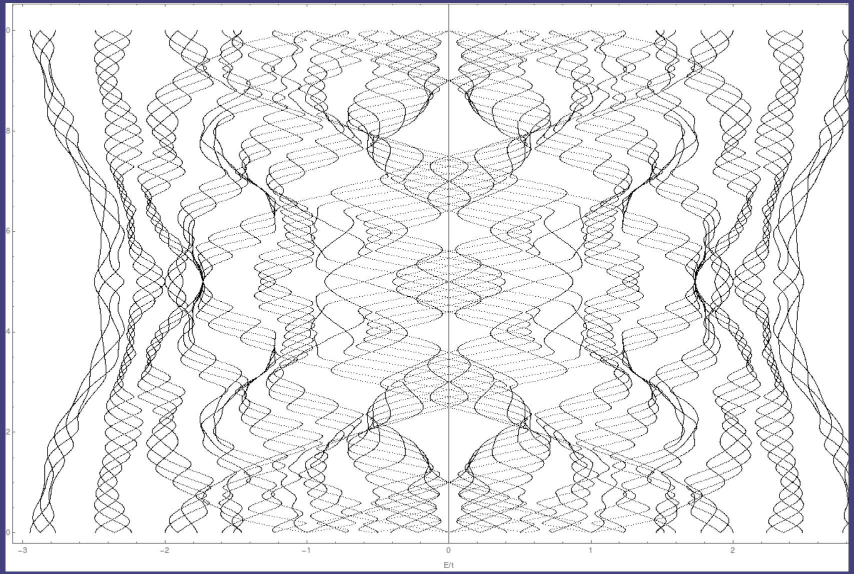


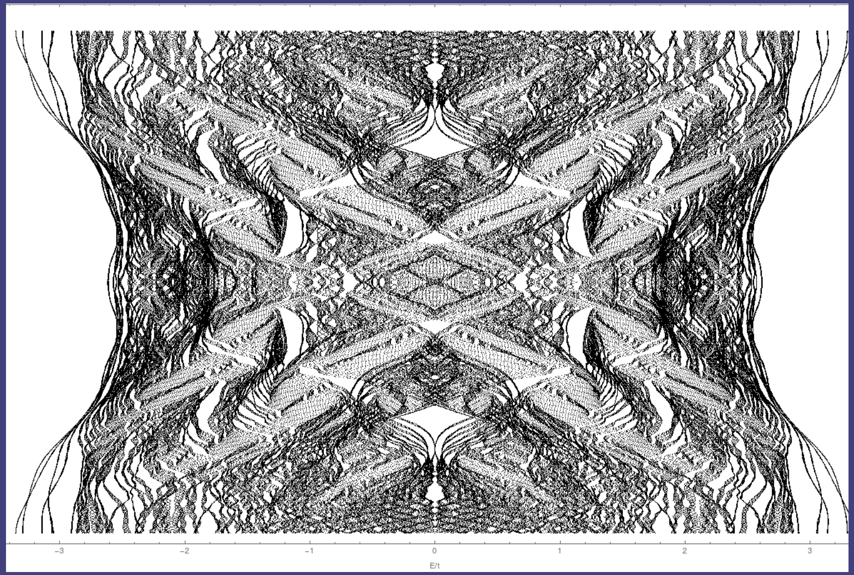


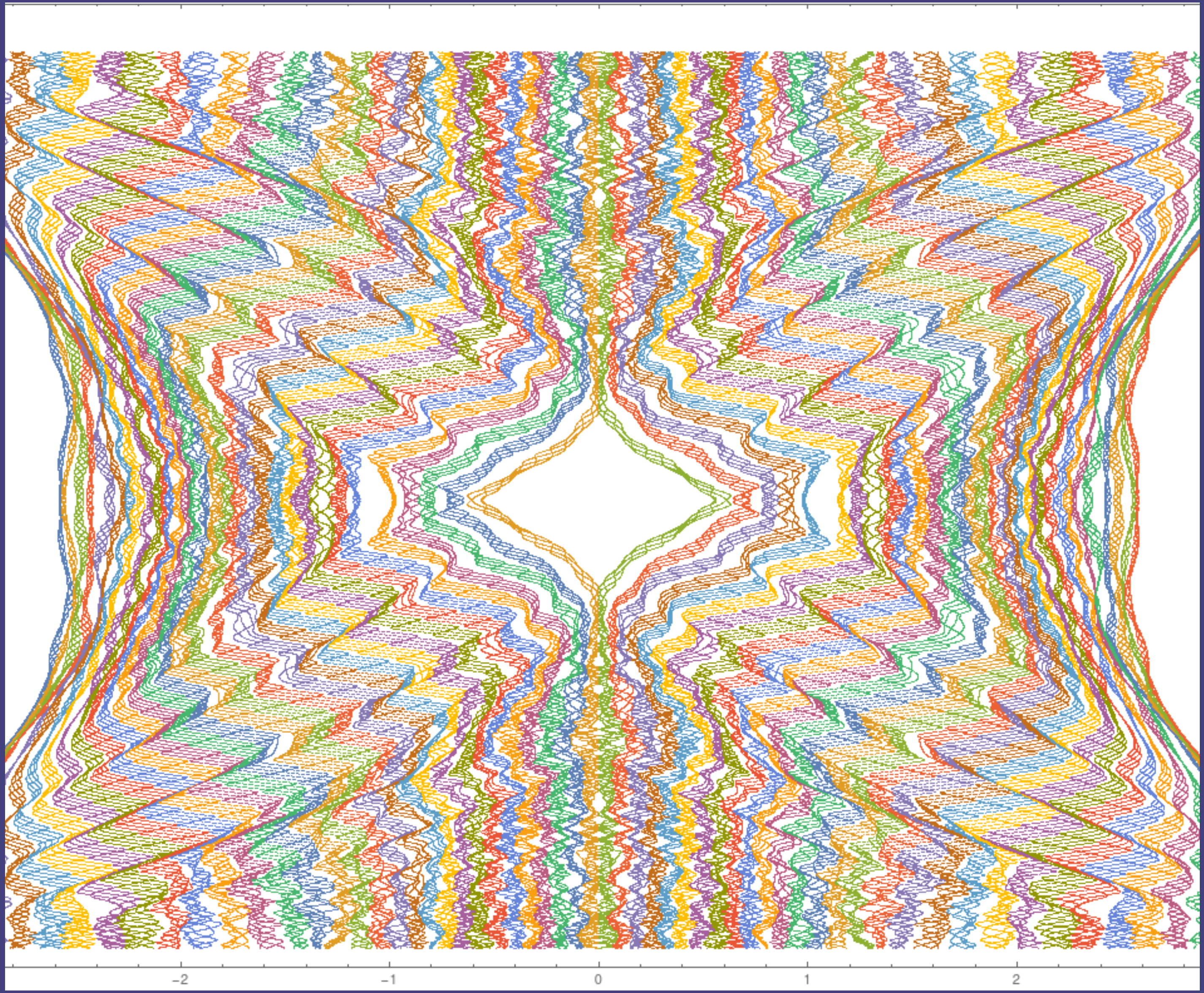


Where the "it could be a zero or a one… at the same time" idea comes from

Learning programming





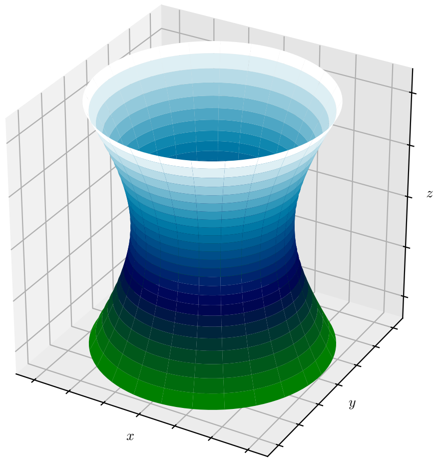

−2
−1
0
1
2

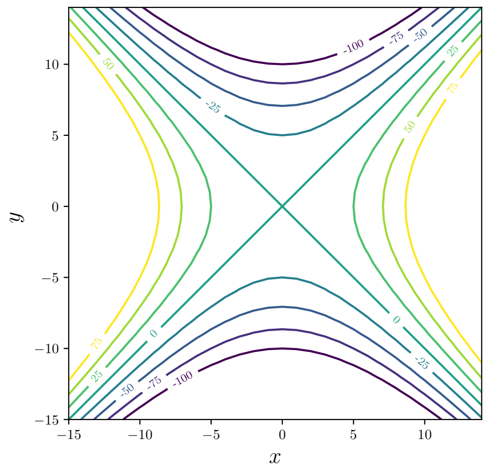
Linear algebra

And lots more!

My favourite project

- My favourite project was in non-Hermitian quantum theory
- I spent a lot of time thinking about what quantum systems are in a purely mathematical way, what conditions can create quantum systems
- Lots of playing with matrices
- This is what I studied for my thesis in my final year, supervised by Dr Eva-Maria Graefe





Postulates of Quantum Mechanics

- Quantum mechanics is a mathematical framework for the development of physical theories
- There are six postulates of quantum mechanics
- These postulates provide a connection between the physical world and the mathematical formalism of quantum mechanics

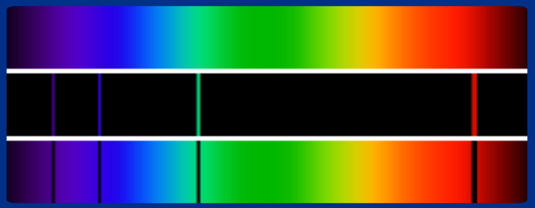
Hermiticity in quantum mechanics

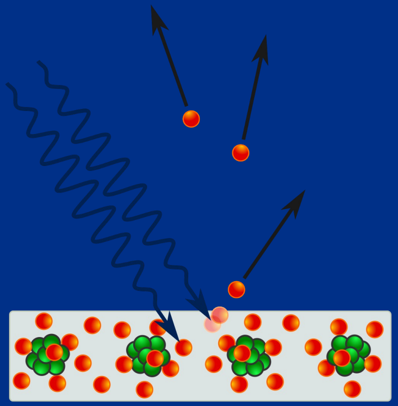
- Hamiltonian operators are used to describe observable properties of particles
- These Hamiltonians (matrices) are Hermitian, and have real eigenvalues

Mathematical formalism

$\longleftrightarrow$

What we see in the real world





Hermitian Hamiltonians look like this

$$\begin{bmatrix} 5 & 1 & 3i \\ 1 & 5 & 1 \\ -3i & 1 & 5 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 3+4i \\ 3-4i & 2 \end{bmatrix}$$

$$H = \begin{bmatrix} x_1 & z_1 & z_2 \\ \overline{z_1} & x_2 & z_3 \\ \overline{z_2} & \overline{z_3} & x_3 \end{bmatrix}$$

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

$$\begin{bmatrix} 1 & 0 & i+j+k \\ 0 & 1 & 0 \\ -i-j-k & 0 & 1 \end{bmatrix}$$

Hermitian Hamiltonians have real eigenvalues

$$\begin{bmatrix} 5 & 1 & 3i \\ 1 & 5 & 1 \\ -3i & 1 & 5 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 3+4i \\ 3-4i & 2 \end{bmatrix}$$

$$H = \begin{bmatrix} x_1 & z_1 & z_2 \\ \overline{z_1} & x_2 & z_3 \\ \overline{z_2} & \overline{z_3} & x_3 \end{bmatrix}$$

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

$$\begin{bmatrix} 1 & 0 & i+j+k \\ 0 & 1 & 0 \\ -i-j-k & 0 & 1 \end{bmatrix}$$

In the 1960s, Dyson classified Hermitian matrices according to what time-reversal symmetries they had

Freeman Dyson in 1963. Source: The New York Times

Time reversal symmetries

What does this mean for H?

1. H has a symmetry A if $[H, A] = HA - AH = 0$.
2. When we act twice with the time-reversal operator $\mathcal{T}$, we return to the same state. $\mathcal{T}^2 |\phi\rangle = \pm |\phi\rangle$.
3. Different entries in H determine if H has even, odd or no time-reversal symmtery.

Types of matrices

1. $[H, \mathcal{T}] = 0$ and $\mathcal{T}^2 = +1 \implies H$ is real $\implies$ modelled by Gaussian Orthogonal Ensemble
2. $[H, \mathcal{T}] = 0$ and $\mathcal{T}^2 = -1 \implies H$ is made up of quaternionic blocks $\implies$ modelled by Gaussian Symplectic Ensemble.
3. $[H, \mathcal{T}] \neq 0 \implies H$ modelled by the Gaussian Unitary Ensemble.

Random matrices

"An ensemble of systems in which all possible laws of interaction are equally probable" – F. J. Dyson

$$\text{GOE} \quad H = \begin{bmatrix} h_1 & h_2 \\ h_2 & h_3 \end{bmatrix}$$

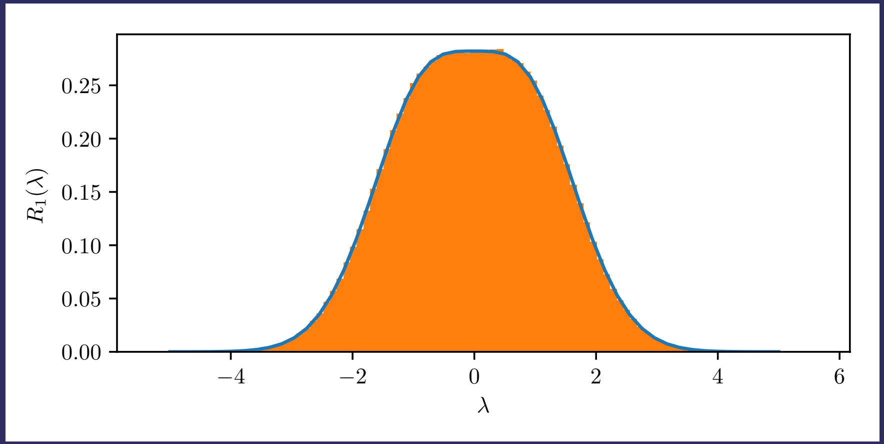
$$\text{GUE} \quad H = \begin{bmatrix} h_1 & h_2^R + ih_2^I \\ h_2^R - ih_2^I & h_3 \end{bmatrix}$$

$$\text{GSE} \quad H = \begin{bmatrix} h_1 & h_2^R + ih_2^I + jh_2^J + kh_2^K \\ h_2^R + ih_2^I + jh_2^J + kh_2^K & h_3 \end{bmatrix}$$

Generate parameters randomly

→

Get eigenvalue statistics



Often diagonalize matrices to read their eigenvalues

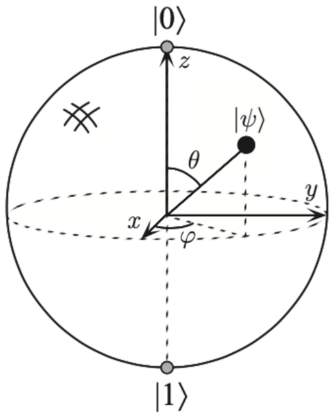
GOE

$$U = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

GUE

$$U = \begin{bmatrix} \cos\theta & -e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & \cos\theta \end{bmatrix}$$

$$\Lambda = U^{-1} H U$$



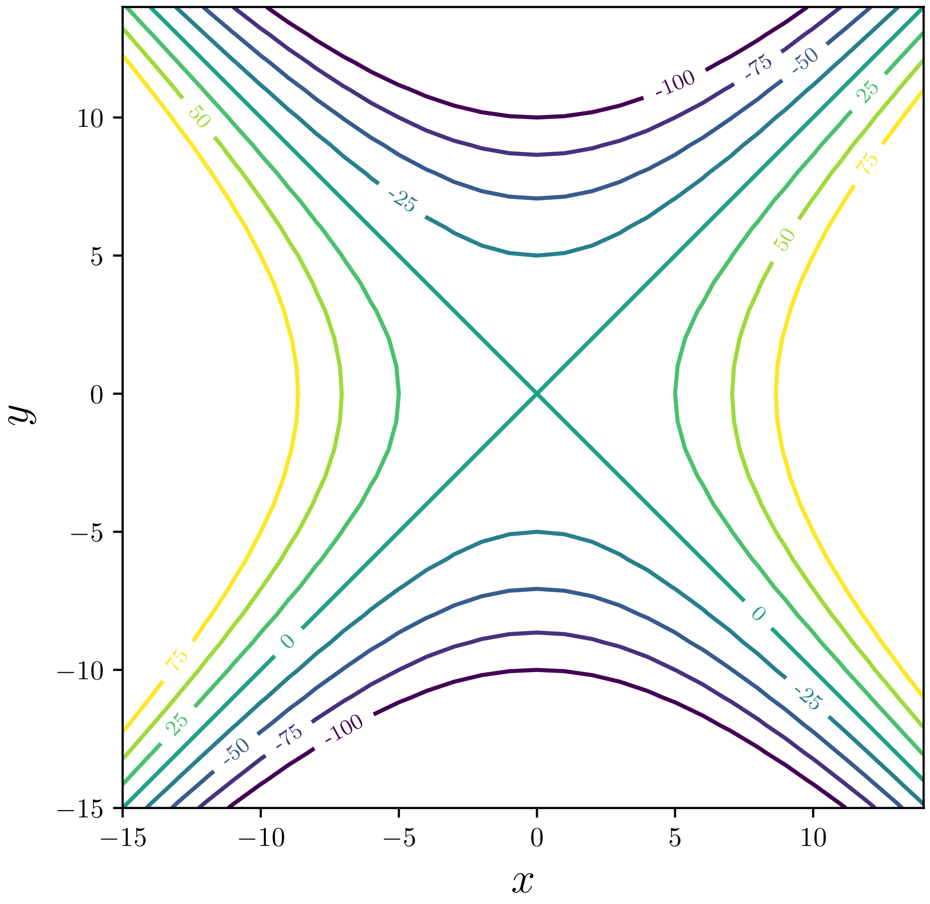
New ensembles

- Mentioned earlier that Hermitian Hamiltonians have real eigenvalues, always
- Not all Hamiltonians are Hermitian!
- PT-symmetric systems can have complex-conjugate eigenvalues
- One-to-one correspondence has been made between PT -symmetric Hamiltonians and new, split-Gaussian ensembles.

Split-complex numbers

- A split-complex number has two parameters x and y, written as $z = x + jy$
- Has indefinite norm

$$|z|^2 = x^2 - y^2$$



Split-complex Hermitian matrices

- Consider Hamiltonian

$$H = \begin{bmatrix} x_1 & x_2 + jy_2 \\ x_2 - jy_2 & x_3 \end{bmatrix}$$

- Has eigenvalues

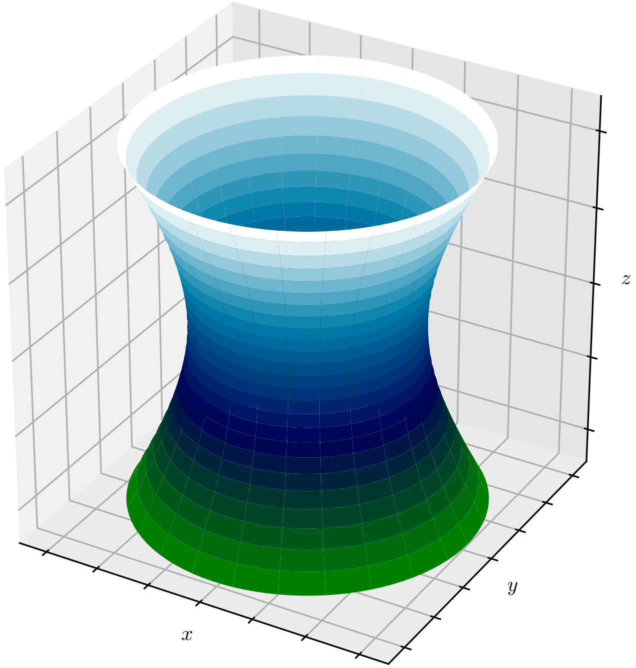
$$\lambda_\pm = \frac{x_1 + x_3 \pm \sqrt{(x_1 - x_3)^2 + 4(x_2{}^2 - y_2{}^2)}}{2}$$

which can either be real or come in complex-conjugate pairs.

Can diagonalize these matrices

Eigenvectors for these systems live on a hyperboloid, rather than a sphere!

$$U = \begin{bmatrix} \cosh\phi\cos\theta + j\sinh\phi & -\cosh\phi\sin\theta \\ \cosh\phi\sin\theta & \cosh\phi\cos\theta - j\sinh\phi \end{bmatrix}$$



$$\Lambda = U^{-1}HU$$

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My work today

What is the Hartree Centre?

- World-leading supercomputing, data analytics, AI and quantum computing technologies
- 120+ scientists, technologists and business professionals in bespoke teams working on challenge-led projects
- UK Government funded to boost productivity and innovation for industry and public sector organisations of all sizes
- Part of the Science and Technology Facilities Council in UK Research and Innovation
- Working with an international network of research communities and technology partners

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Quantum projects

Routing Warehouse Robots

- A quantum/classical hybrid solver was applied to routing robots in Ocado's Customer Fulfillment Centers.
- Combining these two computing paradigms to produce a better solution than would be possible if used in isolation.
- After considering trans-Atlantic communication, quantum annealing approach starts to become competitive.

ocado TECHNOLOGY

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+

D:WAVE

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AA-B03
AA-A77
AA-A41

Quantum Optimization for Routing

Team: Vendel Szeremi, Julien Gacon, Dariusz Lasecki, Daniel Egger, Luciano Bello, Stefan Woerner

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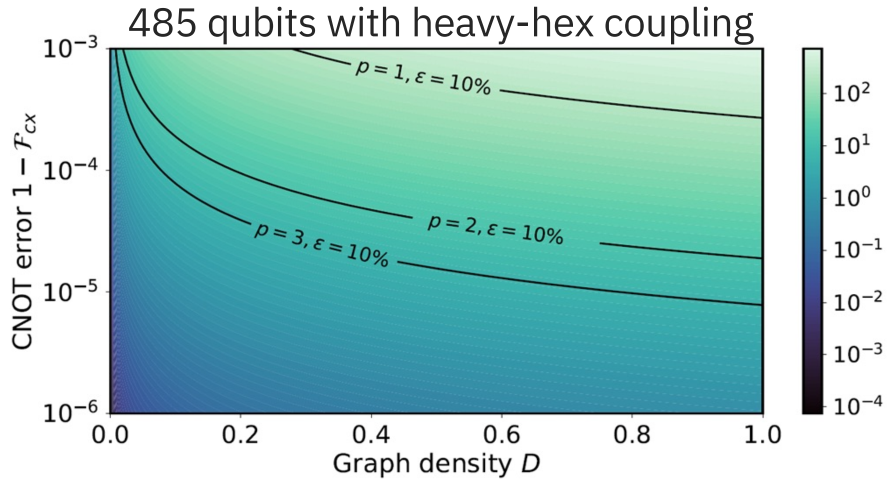
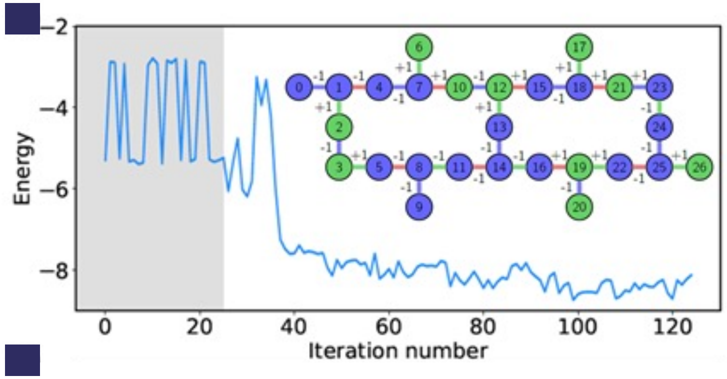
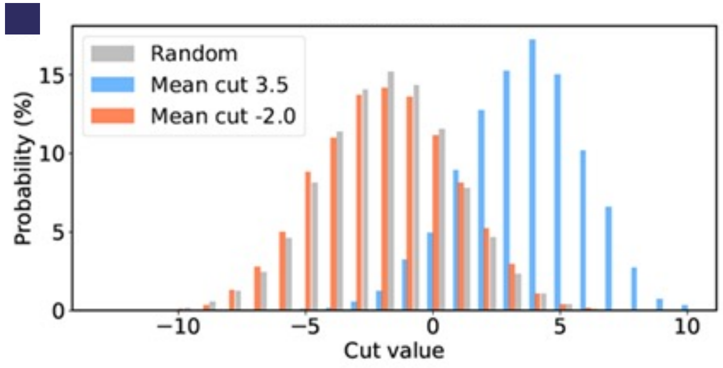
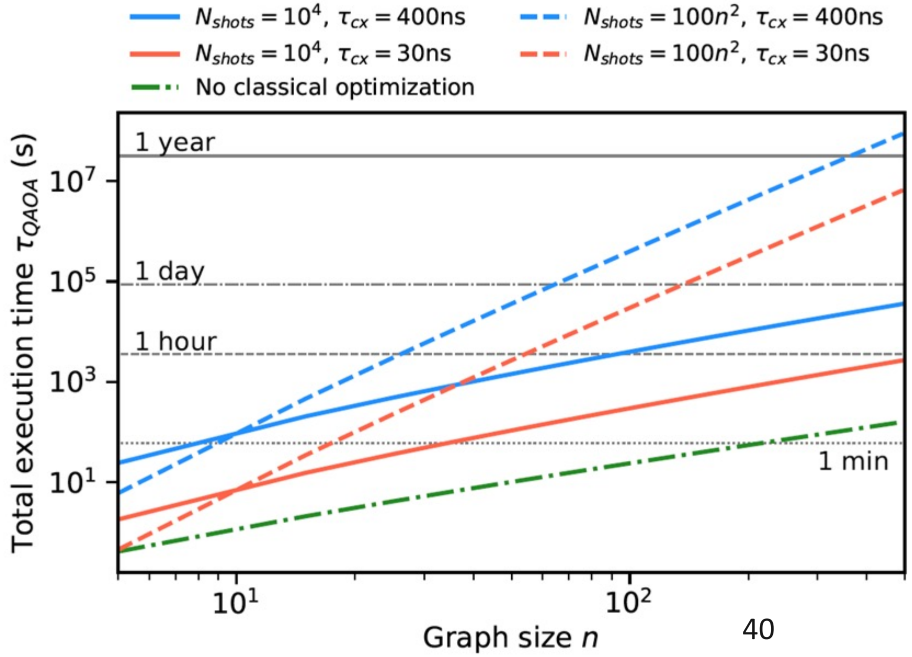
IBM **Quantum**

- Developed SWAP strategies
  ==⇒ Overcome limited device connectivity.
- Evaluated gate fidelity criteria for the SWAP strategies
  ⟹ When does it make sense to run on noisy hardware?
- Estimates of execution time on quantum hardware
  ⟹ Identify bottlenecks.
- Qiskit QAOA Runtime
  ⟹ Explore QAOA at scale.









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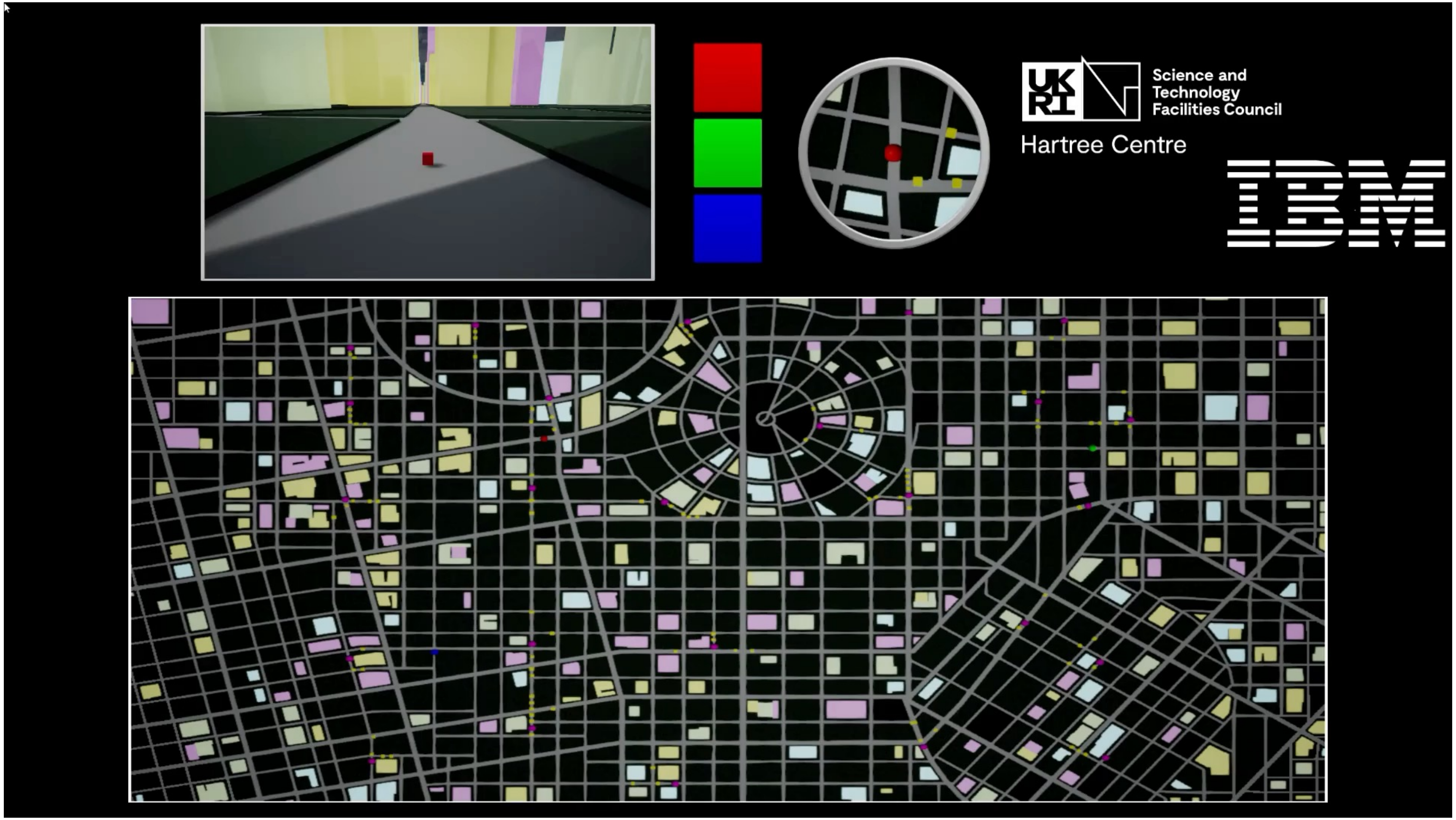
Paper: “Scaling of the Quantum Approximate Optimization Algorithm”
arXiv:2202.03459



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QML Framework for Virtual Screening in Drug Discovery

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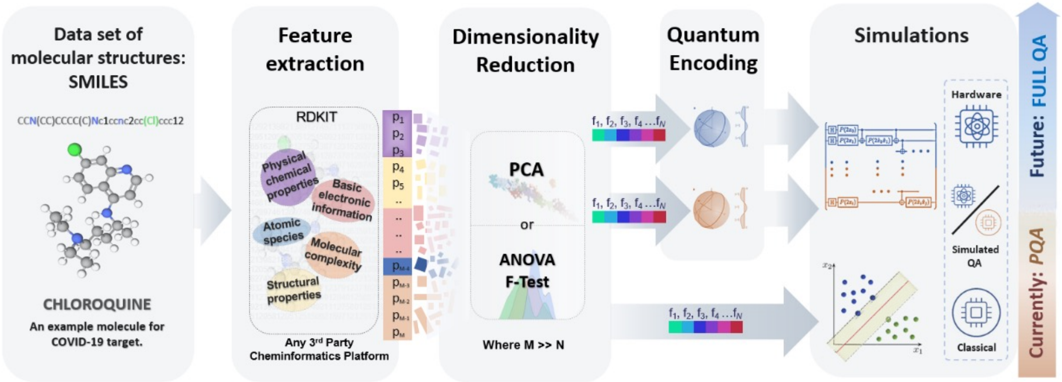
IBM **Quantum**

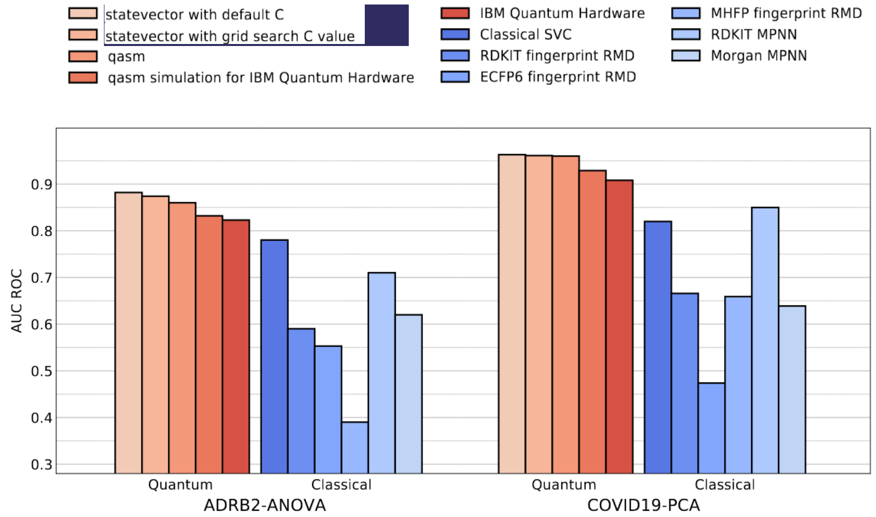
Team: Stefano Mensa, Emre Sahin, Francesco Tacchino, Panagiotis Kl. Barkoutsos, Ivano Tavernelli



Prospective Quantum Advantage: we observe instances in which simulated quantum algorithms and proof-of-principle hardware experiments on a reduced number of features outperform classical methods in the same conditions. No evident restrictions to the extension to larger problem sizes.

Virtual screening: searching digital libraries of molecules to identify structures which are most likely to bind to a drug target.

- Interface QML functionalities in Qiskit with cheminformatics tools (RDKit): automated and integrated workflow
- Investigate a novel practical use of quantum kernel methods using classical molecular data/descriptors
- Assess the potential for quantum advantage, supporting it with empirical evidence
- Experiments (8 qubits) on IBM Quantum Montreal and Guadalupe
- Contribution to Qiskit Nature and ML



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Paper: "Quantum Machine Learning Framework for Virtual Screening in Drug Discovery: a Prospective Quantum Advantage", arXiv:2204.04017

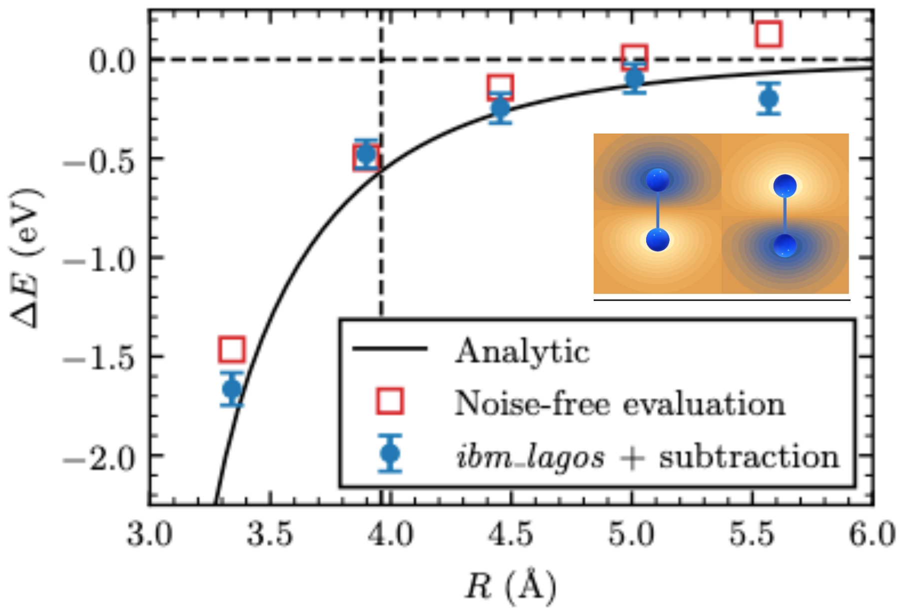
Weak intermolecular interactions on quantum processors

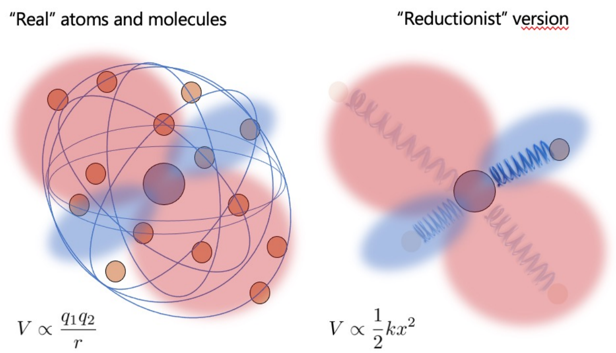
Team: Lewis W. Anderson, Martin Kiffner, Panagiotis Kl. Barkoutsos, Ivano Tavernelli, Jason Crain, Dieter Jaksch

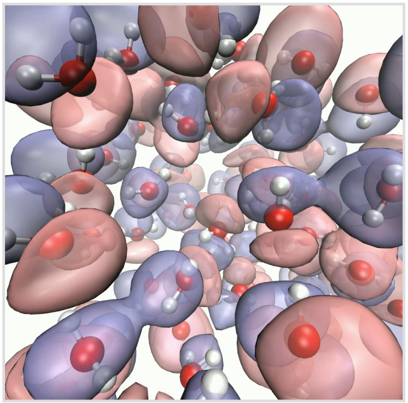
- We developed a coarse-grained representation of the electronic response that is ideally suited for determining the ground state of weakly interacting molecules using a VQA.

➔ qubit resource grows linearly with the number of molecules

- We derived scaling behaviour for the number of circuits and measurements required, which compare favourably to traditional variational quantum eigensolver methods.
- Demonstrated on IBM hardware
- Corresponding Qiskit module in preparation







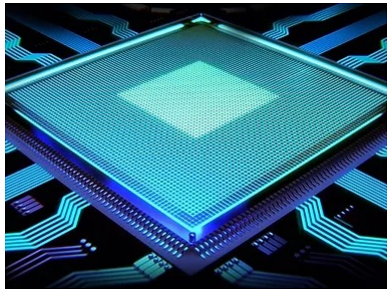
London Dispersion Forces: weak, non-covalent, molecular interactions which are particularly difficult to capture ab-initio using conventional electronic structure methods such as DFT.

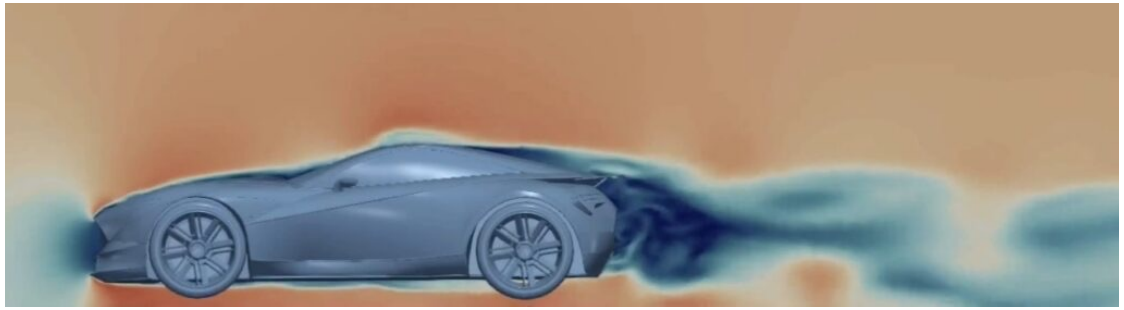
Paper: "Coarse grained intermolecular interactions on quantum processors", Physical review A (in press, 2022).

Quantum Error Correction

https://www.qecproject.co.uk

- Using quantum algorithms to solve problems in computational fluid dynamics
- Currently using Hartree's ATOS Quantum Learning Machine
- Our work to be used as a test case to build the first cloud-accessible, error-corrected, scalable quantum computer





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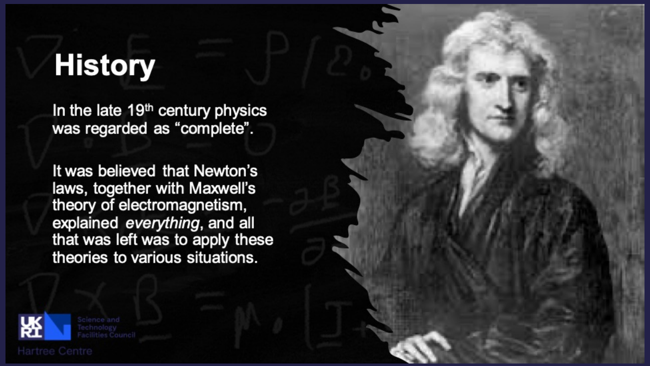
Learning Opportunities

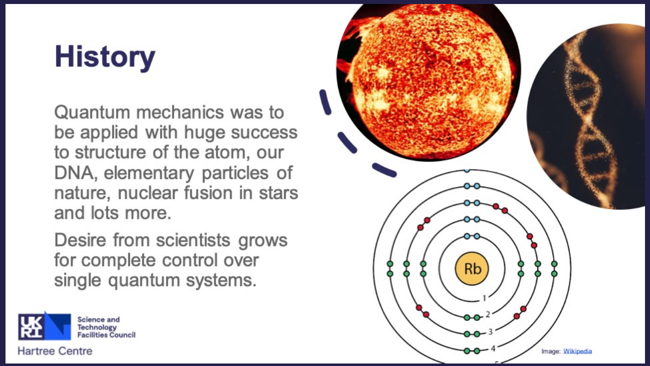
EXPLAIN Training Courses

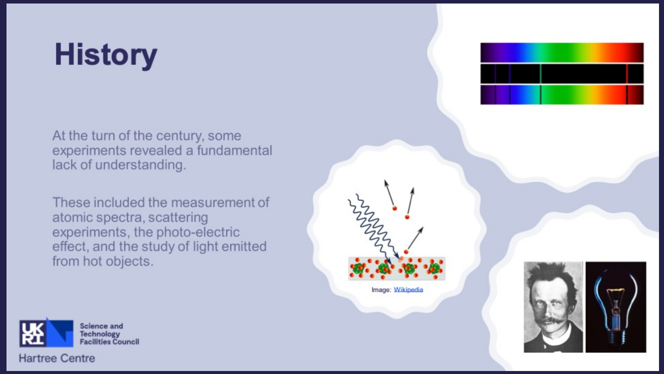
Accessible supercomputing, data science and AI training with industry in mind

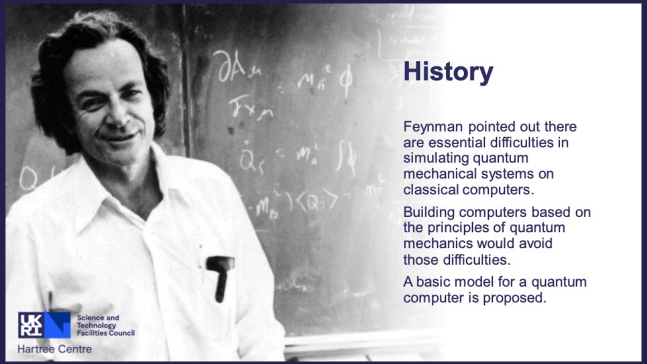
Designed to enable individuals, businesses and public sector organisations to take advantage of digital technologies like supercomputing, data science, AI, full stack, cloud and quantum computing

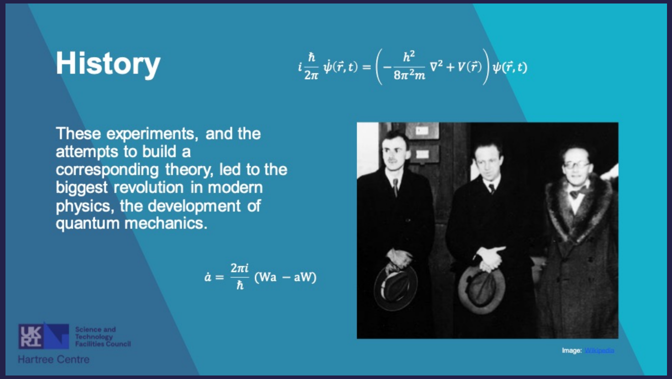
Beginner's Guide to Quantum Computing

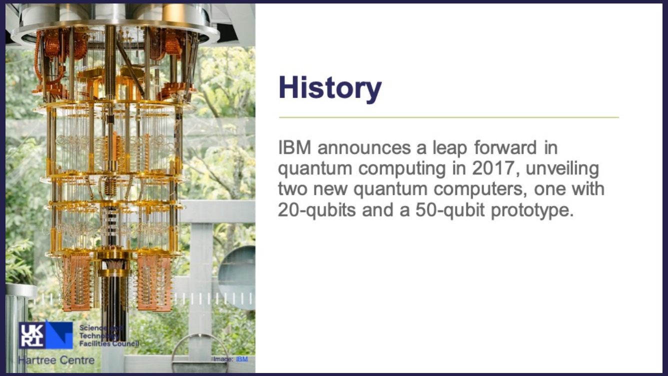












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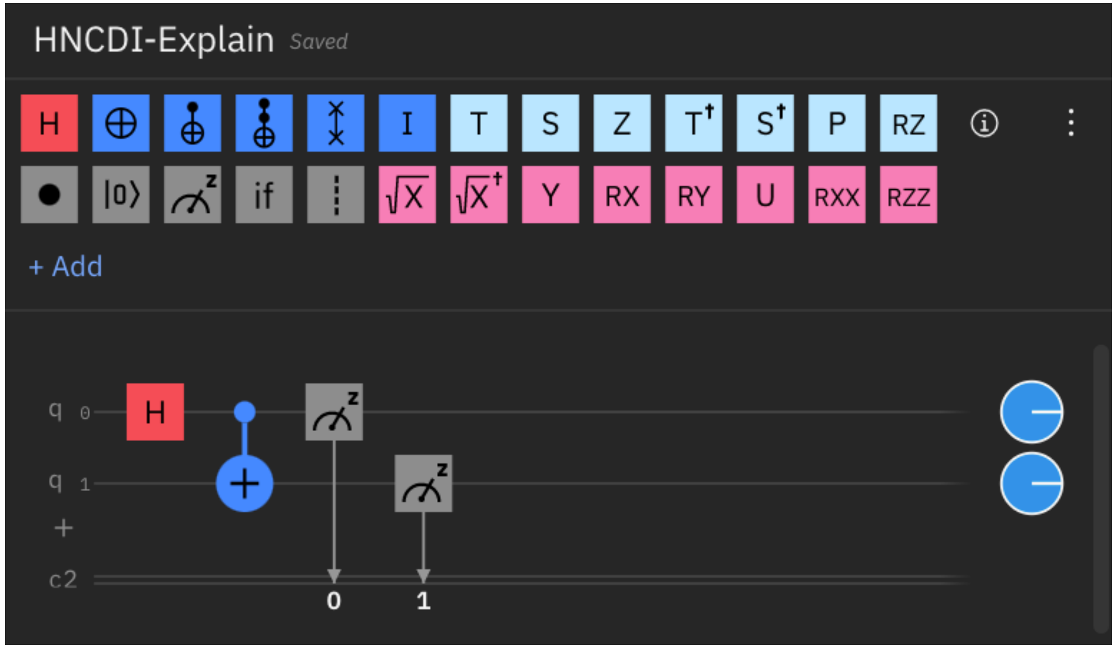
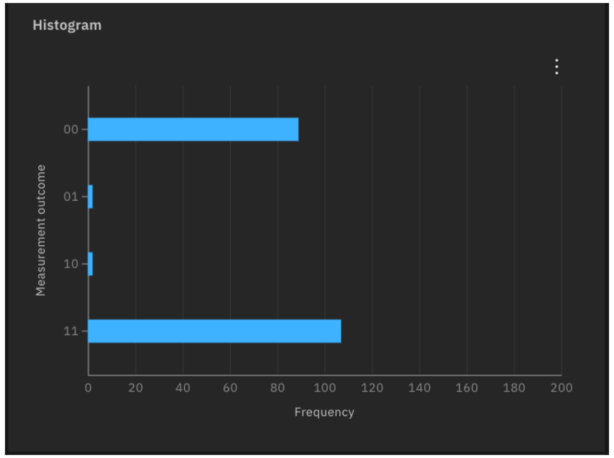
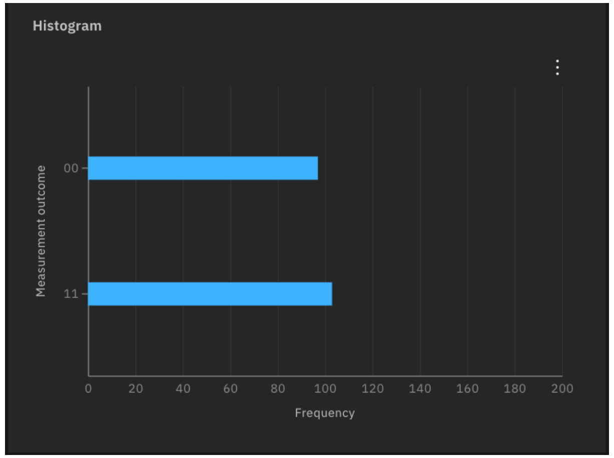
Beginner's Guide to Quantum Computing







Explain Quantum Courses

- Beginner's Guide to Quantum Computing
- Practical Guide to Quantum Computing
- Fundamentals of Quantum Computing

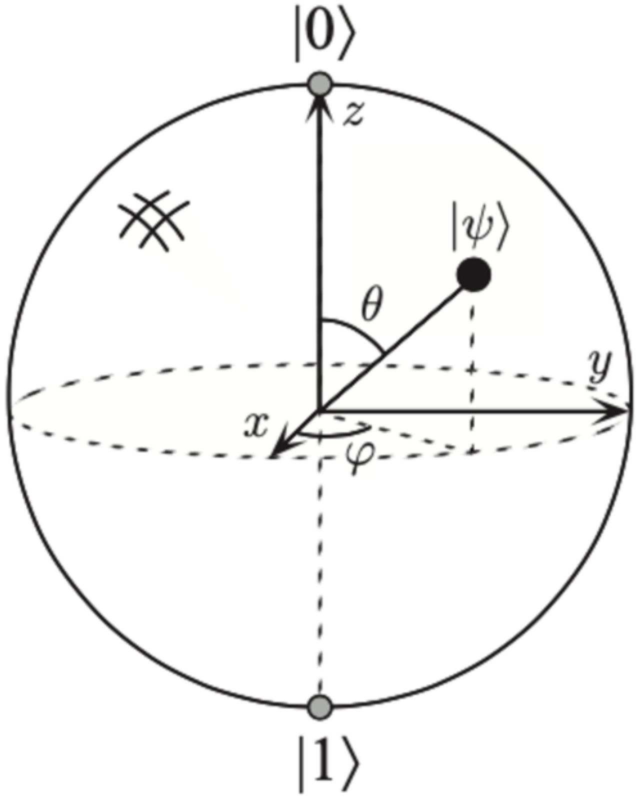


Figure: p.15 of [Quantum Computation and Quantum Information, Nielsen and Chuang]

Other EXPLAIN courses – all free!

- Beginner's Guide to High Performance Computing
- Introduction to Data Collection and Preparation
- Beginner's Guide to Cloud for Industry
- Beginner's Guide to Machine Learning and Data Science
- Beginner's Guide to Artificial Intelligence
- Beginner's Guide to Modelling
- Beginner's Guide to Quantum Computing
- Beginner's Guide to Exascale Computing
- Beginner's Guide to Data Visualisation
- Beginner's Guide to Natural Language Processing
- Demystifying Data Engineering
- Practical Guide to Cloud: Onboarding with Azure
- Infrastructure as Code in the Cloud
- Practical Guide to High Performance Computing
- Mixed Language Programming: Calling C from Python
- Deploying and Testing Software-as-a-Service Applications
- Mathematical Fundamentals of Quantum Computing
- Practical Guide to IoT
- Machine Learning Defining Problem Scope and Assessing Model Requirements
- Performance Analysis Tools for Hartree Centre Systems
- Supercharge your Cloud Development Workflow: Introduction to Docker and GitHub Actions for ML Apps
- How to Scale Up your Company's Code
- Patterns of Concurrency and Parallelism for Commodity Servers
- Practical Guide to Neural Networks and Deep Neural Networks
- Fundamentals of Scientific Data Analysis Workflows and Pipelines
- Advancing Data Science Solutions
- Novel Software Environments for Exascale Computing
- Practical Guide to Reinforcement Learning
- Quantum Computing – the next level

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Other resources I like to use:

- ‘Quantum Computation and Quantum Information’, Nielsen and Chuang
- Qiskit textbook

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Questions?

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Thank you

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