Quantum Computing & Applications for Engineering

9/10/2024

Today’s Goals

1. Get oriented:
    a. Understand what this course is about.
    b. Understand what the quantum technology field is about.
2. Set up and run your first quantum programs.
    a. Python environment
    b. IBM Accounts & first programs

Agenda

- Part 1 - Lecture
  - Introduction & Course Overview
  - Course Policies & Logistics
- Part 2 - Breakout
  - Guest speaker: Mike Sofka, RPI QED Team
  - Environment setup
  - Running your first program
- Part 3 - Regroup
  - Discuss HW
  - Continue setup
  - Free discussion

Why This Course?

- We have a shiny new quantum computer!
  - What can (and can't) we do with it?
  - How do we program it?
- We're starting from a blank slate!
  - First university with unlimited, low-friction access to a quantum machine
  - Opportunities for new perspectives
- Quantum is more than computing!
  - Sensors
  - Networks
  - Supporting technologies

The new machine on the day of the ribbon cutting ceremony.

About Me

- Attended RPI 2006-2016
  - Nuclear engineering bachelor’s & PhD
  - Experimental work at LINAC and RCF
  - Greek life, American Nuclear Society
- Currently at NNL/KAPL in Schenectady
  - Future technology group
  - Started quantum work ~2017
  - Projects include quantum computing, sensing and materials
  - Check us out at the career fair!
- Connected with several quantum communities & organizations
  - Industry, academia, government, nonprofit
  - Let me know your interests!

*All opinions expressed are my own and not those of any other organization.

Course Goals

- Get familiar with using real quantum hardware.
  - Learn quantum computing as it exists today.
  - Understand the capabilities, limitations and potential.
  - Perform hands-on experiments with the machine.
- Build awareness of quantum applications and technologies.
  - Other kinds of qubits
  - Sensors & networks
  - Application areas
  - Supporting technologies (lasers, cryogenics, electronics)
- Understand the research, career, and business opportunities in quantum technologies.

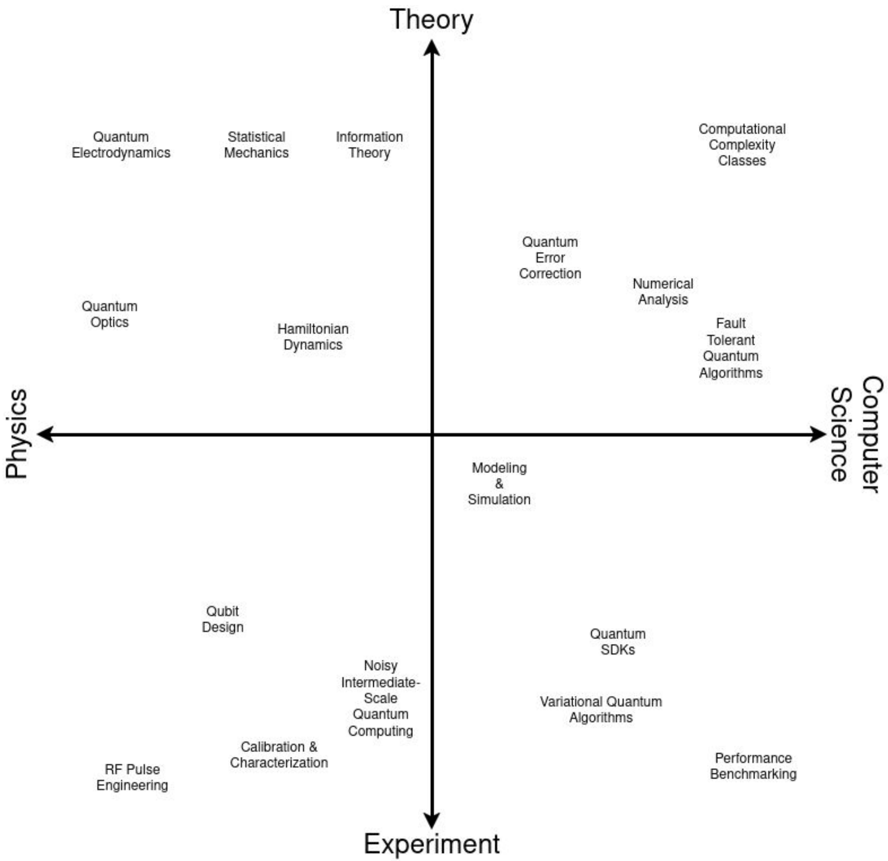
Why is this course different?

- This is one of the few quantum courses (the first?) with <u>unlimited</u> hardware access.
  - Innumerable courses on math, physics, and theory
  - Lots of online tutorials with simulators and more limited hardware access
- We're approaching it as engineers, not physicists or computer scientists.
  - "User-side" perspectives
  - Application-oriented focus
- We're treating imperfections from the start.
  - Idealized treatments of quantum information require "unlearning" some assumptions.
  - We'll come from the other side and learn how we can fight for perfection.
- We consider other technologies.
  - Different qubit modalities.
  - Adjacent and spinoff technologies.

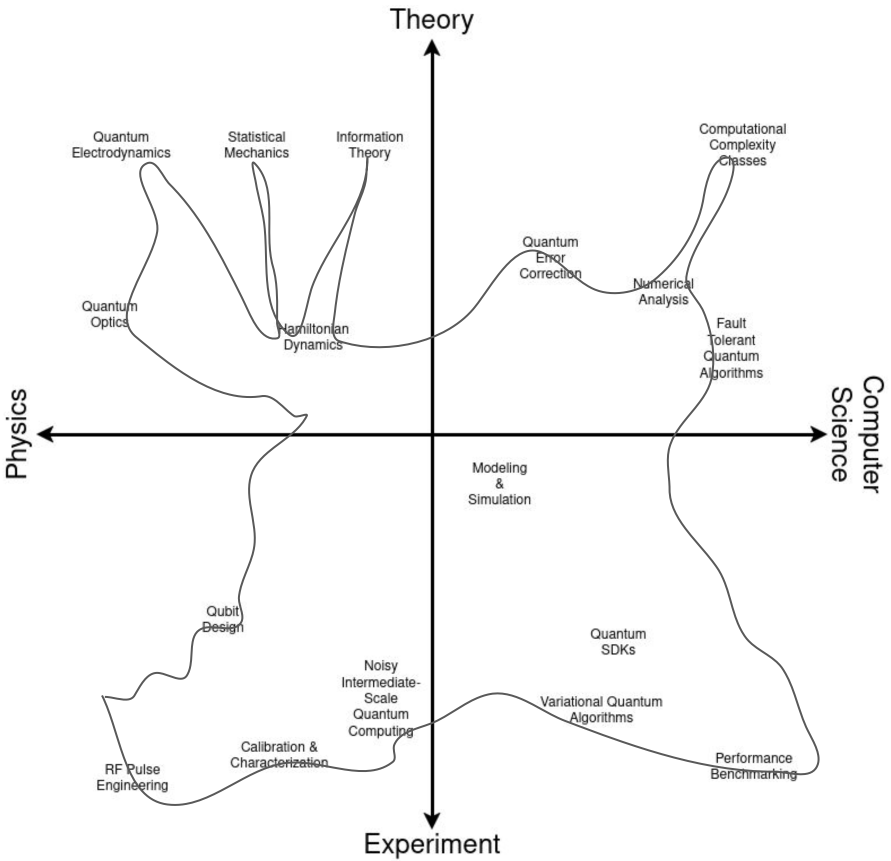
What's in this course

- Basics of qubits, gates, and circuits
  - Enough physics and linear algebra to be dangerous
  - Programming using IBM Qiskit
- Understanding the hardware
  - Different qubit modalities and how they work
  - Characterizing performance and noise sources
  - Mitigating the effects of noise
- Technology landscape
  - Industry and research opportunities
  - State-of-the-art in contemporary research
- Survey of applications in science & engineering

What’s in this course

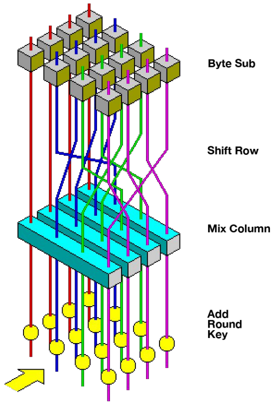


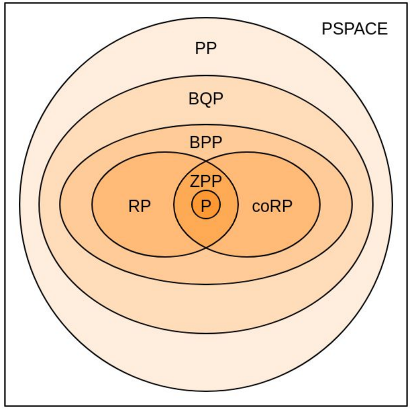
What’s in this course

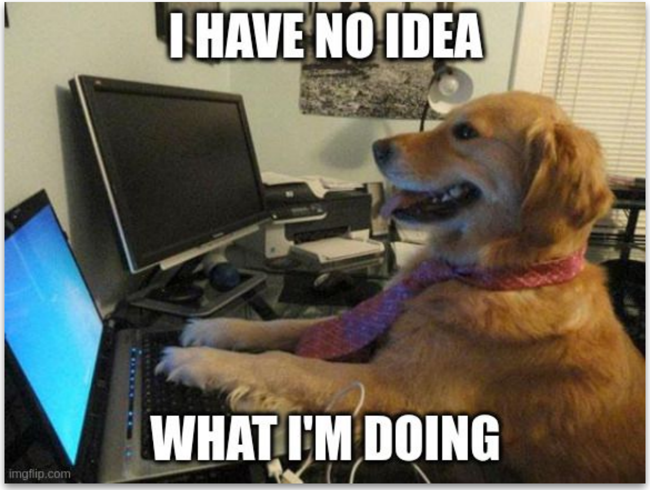


What's not in this course

- Detailed things that already have (or would need) their own in-depth courses:
  - Fault-tolerant quantum computing theory
  - Detailed hardware physics
  - Theoretical computer science & complexity
  - Cryptography & cybersecurity
- Introductory Python programming
  - Basic proficiency is assumed (loops, conditionals, functions, classes).
  - We don't have time to cover the basics, but you're encouraged to learn as you go
  - Drop, audit, P/NC, or get help if you think you will struggle.







Course Philosophy

- Guided discovery
  - Instructor defines a goal
  - Students pursue that goal by whatever means necessary
  - Instructor acts as a knowledgeable guide
- Breadth vs. depth
  - Quantum is a huge and fascinating field that changes daily
  - Too-narrow focus risks obsolescence
- Hacker Mindset
  - Learn by doing
  - Build mental models and understanding as we go
- Sit back, relax, and enjoy learning!

Logistics & Policies

General Logistics

- Email: mcderb2@rpi.edu or bjmcder@gmail.com (cc both for visibility)
- TA: Chris Stamopoulos (stamoc@rpi.edu)
- Phone:
    - 978-760-2359 (after 4pm or before 8am, text preferred)
    - 518-612-5016 (desk line during work hours if urgent)
- Office hours: Friday 10:30-11:30 or by appointment
- Reading Materials
    - No textbook - there aren't any (yet) that deal with practical hardware usage.
    - Videos, articles, and papers will be provided to accompany homework assignments.
    - Optional and recommended resources are listed
- LMS Page
    - Central source of truth for grades, assignments & schedules
    - Location for homework submissions

In-Class Format

- 4-7pm on Tuesdays
  - Bring your laptops
  - Bringing food/drink is ok
- Lecture-Breakout-Regroup Format
  - ~45 minutes each with 5-10 minute breaks in-between
  - Lecture: Introduce the topics and goals for the day
  - Breakout: Activities, guest speakers, work on HW, lightning talks, etc.
  - Regroup: Discuss the results of the breakout and next steps
- Missed classes
  - If you have a planned absence, let me know
  - If you’re sick, please stay home
  - If I’m absent, I will email contingency plans

Grading

- 800 possible points
  - 5 homeworks at 100 points each (lowest dropped)
  - 2 projects at 200 points each
  - 10 bonus assignments at 10 points each
- You must attempt every assignment in good faith (e.g. don’t slack once you hit 740)
- Flexibility is intentional

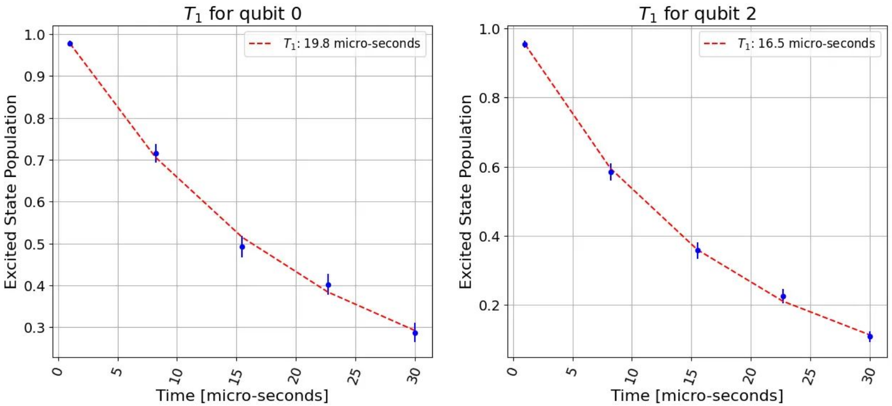
Minimum Required Score	Letter Grade
740	A
720	A-
680	B+
660	B
640	B-
620	C+
600	C
580	C-
560	D+
540	D
< 540	F

Homework

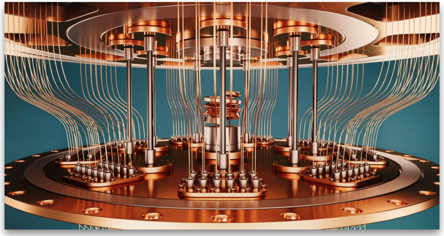
- A mix of calculation, free response, reading & research, and programming exercises.
- Due by <u>11:59pm on Friday</u> of the week indicated in the syllabus.
  - No late work accepted.
  - If there are technical difficulties, let me know.
  - If you have an illness, emergency, or known conflict, please talk to me.
- Redemption opportunities
  - Lowest grade dropped
  - Can correct & resubmit <u>up to two (2)</u> HWs
- Submissions are to be done individually
  - Working in groups is ok and encouraged
  - If you work in a group, please acknowledge who you worked with.

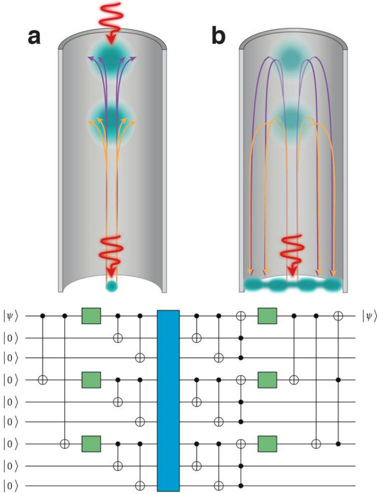
Projects

- Two group projects (worth 2x HW)
- Project 1: Quantum Hardware Characterization & Calibration
  - Perform a full characterization run of the on-campus system
  - Compare your results with the ones IBM provides
- Project 2: Quantum Technology Frontiers
  - Choose or propose a quantum technology, application, software library, company, or research article.
  - Discover the state of the art in the topic you choose, implement a small example on the IBM machine (if applicable).
  - Deliver a written summary and short 10-15 minute demo talk.



Coherence Time Calibration (Qiskit)



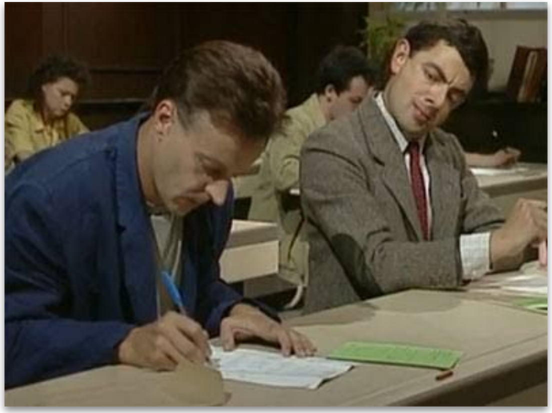


Bonus Assignments

- Each week, you can submit a bonus assignment.
  - Submissions are worth up to 10 extra points.
  - Up to 10 submissions will be accepted.
  - Submit as a <1 page response, a Github repo, or a 2 minute lightning talk in class.
  - Each HW will have a suggested bonus problem.
- Choose from a list:
  - Interview a quantum researcher and learn about their work.
  - Provide a review of a recent research article.
  - Research and review a quantum company, product or service.
  - Critique popular sources (articles, videos, etc.) for accuracy vs. hype
  - Write or demonstrate a mini-app that uses the IBM machine or another quantum device.
- Or propose your own!

Academic Integrity

- There’s no reason to cheat!
- …so please don’t!
    - Pass off work of someone else as your own.
    - Copy work of others without acknowledgement.
    - Pay someone to do your work for you.
    - Blindly copy/paste from outside sources/Stack Overflow/ChatGPT without citation
    - …you know it when you see it.
- Irredeemable penalties:
    - First offense - Automatic zero, cannot be dropped or corrected
    - Subsequent offense - Automatic F for the course
- <u>TL;DR - Cite your sources, acknowledge everything and everyone.</u>



All memes made with https://imgflip.com/memegenerator

Citing Your Sources

- You can use whatever resources you need to do an assignment (unless otherwise specified).
  - Books, articles, proceedings and other scholarly work
  - Videos & tutorials
  - Open source software
  - Discussions with peers & outside experts
- Include a References section in your submitted work.
  - Use whatever style you prefer, just be consistent.
  - RPI library has style guides on their webpage
- When in doubt, over-cite.

ChatGPT, AI, LLMs and all that

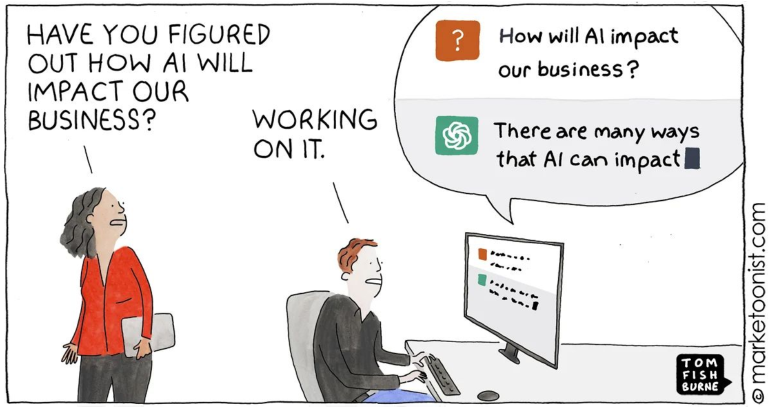
- Use of AI tools is permitted*.
  - You are still responsible for correctness and quality of all work submitted.
  - You must clearly state where and how you used it.
  - You are still held responsible for any plagiarized content.
  - You must still ensure the correctness and relevance of all citations.
- *It probably won’t help in ways you expect.
  - Even factually correct responses can be vague and unenlightening.
  - Citations are frequently wrong, fabricated, or irrelevant.
  - Knowledge of quantum programming tools and research is usually out of date.
  - ChatGPT has an unnaturally fluffy and obtuse writing style.
- Rules of thumb:
  - Use your own brain and your own voice.
  - Always be asking “am I learning, or am I being lazy?”

Claude

AI-generated clipart is always encouraged (Dall-E)

ChatGPT, AI, LLMs and all that

- Encouraged uses
  - Explaining, rephrasing or simplifying complex topics (e.g. from research papers)
  - Spelling & grammar improvements
  - General coding assistance
  - Outlines, summaries
  - Brainstorming, overcoming writer's block
  - Studying the AI itself
- Discouraged uses
  - Generating content for direct submission (please go above and beyond)
  - Complex calculations or derivations
  - Quantum code generation



Don't be this guy!

External Help

- You are encouraged to talk with other quantum experts and researchers.
  - Faculty, staff, postdocs, graduate students at RPI and other universities
  - Staff at IBM and other quantum technology companies
- Acknowledge any external help or discussions.
  - "Schmoe, Joseph. Private Communication. February 31, 2099."
  - "We would like to thank Joe Schmoe at <company/department> for the helpful discussions on <topic>."
- External consultants cannot do work on your behalf.
  - Exception 1: Providing pre-existing datasets that you use in an analysis.
  - Exception 2: Running code on your behalf on a system you cannot access (e.g. supercomputers, non-IBM machines)

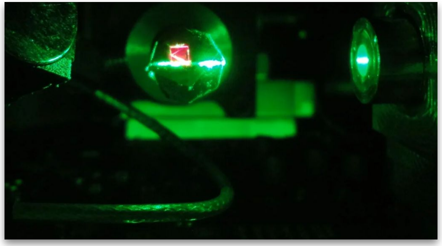
Conduct & Professionalism

- Share your knowledge respectfully.
  - We all have different backgrounds and experiences.
  - We're all still learning (me included).
- Communicate any concerns openly.
  - The material is challenging and changes rapidly.
  - The goal of this class is to inspire interest.
  - We can recalibrate as we go to keep things interesting and enjoyable.
- Engage actively.
  - Class is way more interesting when it's an active discussion.
  - We achieve our goals faster when everyone contributes something.
- Have fun!

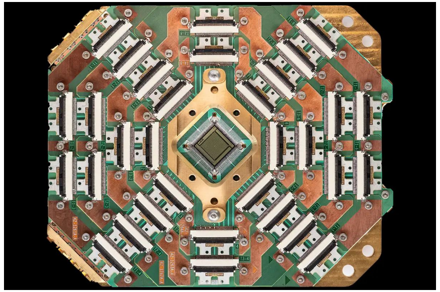
What is Quantum?

What are Quantum Technologies?

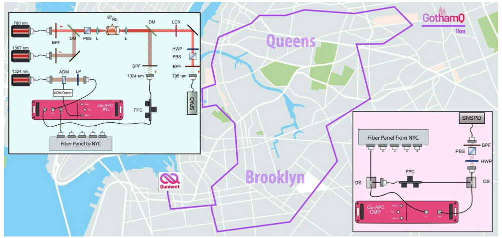
- Any technology that leverages quantum mechanical effects:
    - Superposition
    - Entanglement
    - Tunneling
- We're specifically interested in quantum technologies for measuring, communicating, and processing information.
    - Sensors
    - Networks
    - Computers



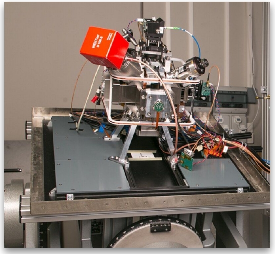
Quantum Diamond Magnetometer (SBQuantum)



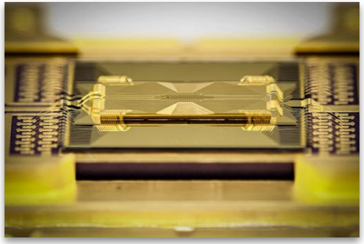
D-Wave Quantum Annealer



Qunnect NYC Quantum Network



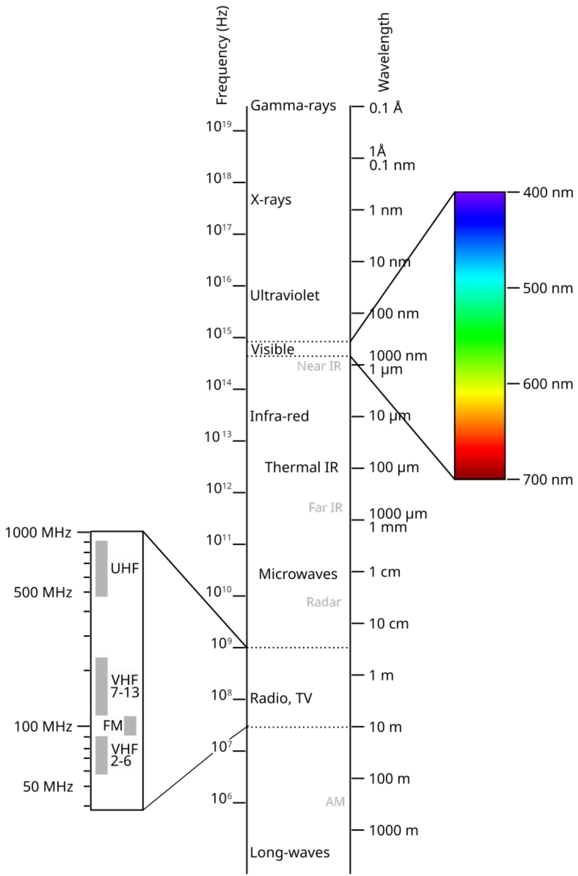
Quantum Navigation System (CNRS)



Ion Trap (IonQ)

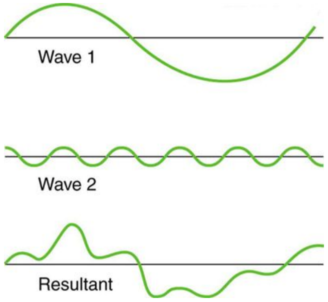
What are they made of?

- Any physical multilevel system:
  - Energy levels in atoms & ions
  - Oscillation modes in superconducting circuits
  - Spins of particles & crystal defects
  - Polarization of photons
- Can be naturally-occuring or engineered
  - Atoms, ions, nuclei, photons
  - CMOS structures, quantum dots, graphene
- Governed by quantum electrodynamics
  - Essentially all manifestations of electromagnetism
  - Microwave to UV ranges

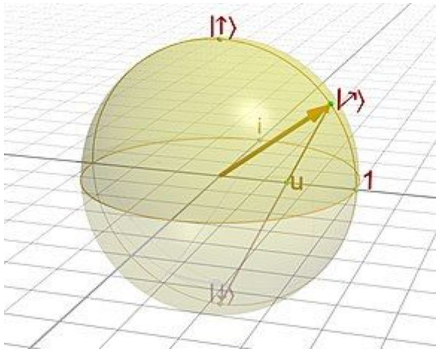


Why Quantum?

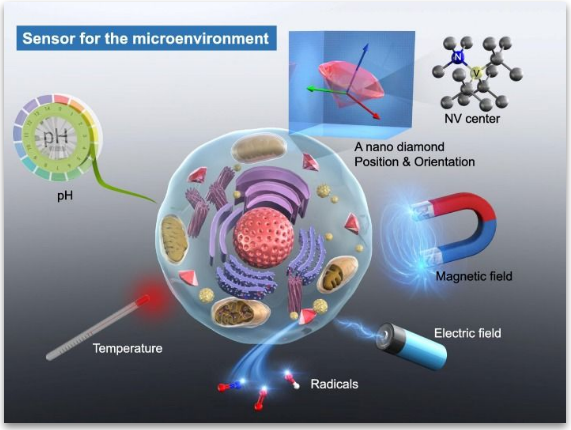
- Compact representations:
  - Superposition lets us combine information compactly.
  - Information is represented as an interacting set of probability amplitudes.
- Large state space:
  - Entanglement lets us grow the space of information we can work with.
  - Exponential amounts of information in a linear number of elements (qubits)
- Useful physical properties:
  - Small size, weight, power consumption, or cost per performance (SWaP-C)
  - Sensitive coupling to environmental parameters (sensors)
  - Immune to copying or eavesdropping (networks)



Superposition of waves



State space of a qubit

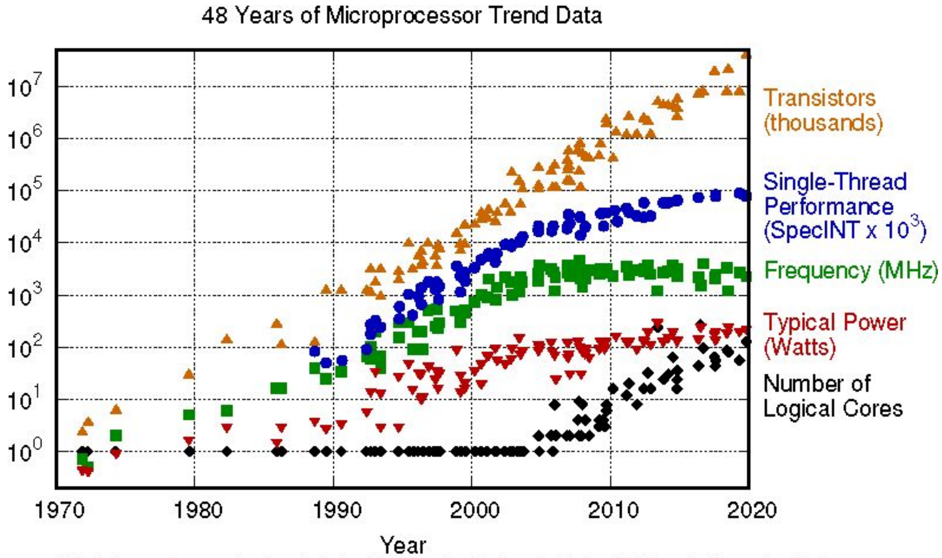


Nanoscale diamond quantum sensors

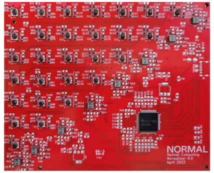
Segawa, Takuya F., and Ryuji Igarashi. "Nanoscale quantum sensing with Nitrogen-Vacancy centers in nanodiamonds–A magnetic resonance perspective." *Progress in Nuclear Magnetic Resonance Spectroscopy* 134 (2023): 20-38.

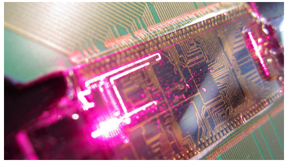
Why Quantum?

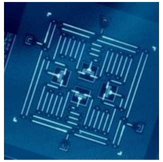
- Computing is on a march towards heterogeneity.
  - CPU performance gains are nearing limits
  - Moore's law not dead, it just went elsewhere
  - The free ride is over
- Specialized accelerators are needed for future performance gains.
  - GPU
  - Quantum
  - Neuromorphic
  - Thermodynamic
  - …
- Quantum is a specific kind of accelerator for "Physics-flavored" problems.



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2019 by K. Rupp

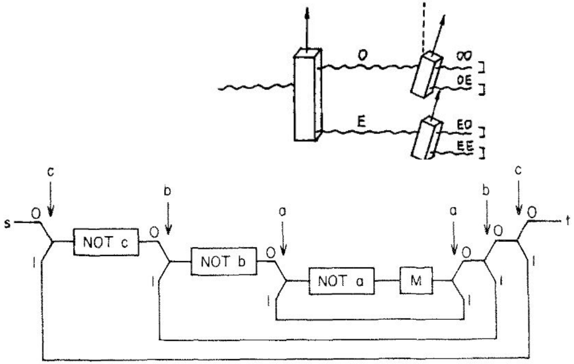




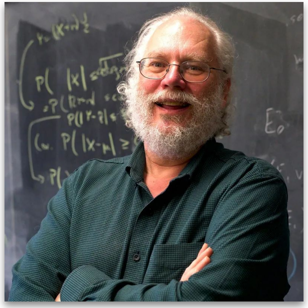


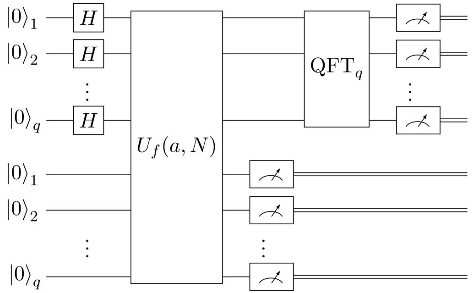
Why now?

- Quantum mechanics has been around a long time.
  - Original theory ~100 years
  - Quantum computing ~40 years
- Shor's Algorithm was the spark that lit the explosion.
  - Proves an efficient way to factor large integers on a quantum computer
  - Critical cybersecurity implications; public-key encryption depends on the presumed difficulty of factoring.
- Initial theories worked out in 90's
  - Error correction & fault tolerance theorems
  - Qubit modalities
- Engineering breakthroughs from the '00s and '10s are yielding rapid growth today.
  - Nanofabrication
  - Photonics
  - Precision Electronics
  - Cloud computing

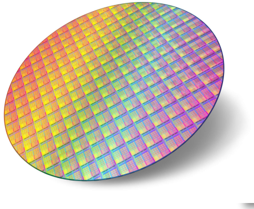


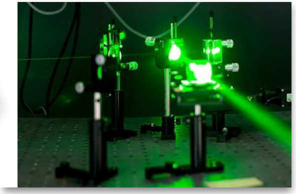
Feynman's original quantum computing concepts [1,2]



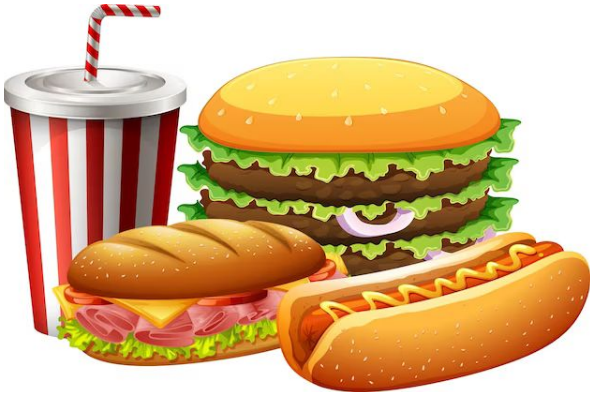


Peter Shor's factoring algorithm [3]





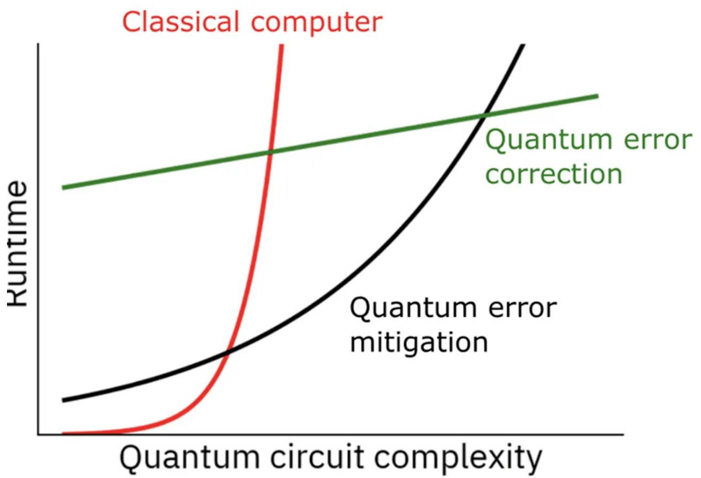
10 Minute Break

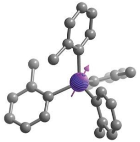


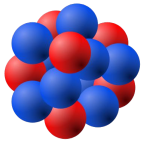
Regroup

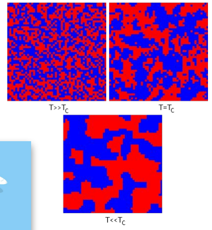
What can it do?

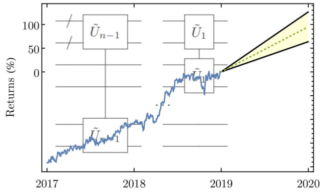
- Quantum computing can improve the scaling behavior of algorithms.
  - Run bigger problems for a given amount of compute resource
  - Run problems that are too big to be tractable.
- Quantum computing is best at specific problems:
  - Strong correlations
  - Probabilistic behaviors
- There are many problems in science, engineering and business that fit this profile.









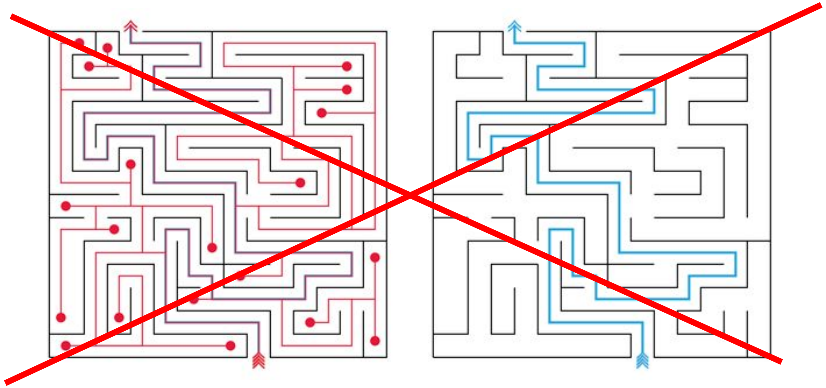


$$E\Psi = \mathbf{H}\Psi$$

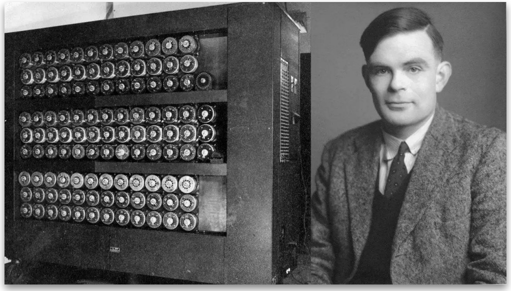
What can't it do?

- Try all the answers in parallel
  - Bad analogy with a glimmer of truth
- Solve every problem exponentially better.
  - Quadratic is always guaranteed (with overhead)
  - Physical "clock speed" is slower
- Replace all classical computers
  - Possible in theory, but undesirable
  - Quantum is another kind of accelerator
- Automatically solve <complex societal problem>
  - Climate change
  - World hunger
  - Political corruption
  - All of cybersecurity
  - Predicting the stock market
  - Artificial General Intelligence
  - …

No!



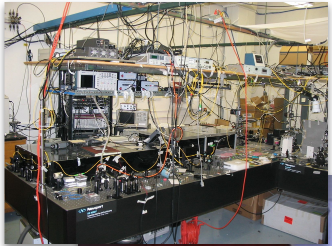
A popular, yet incorrect maze analogy

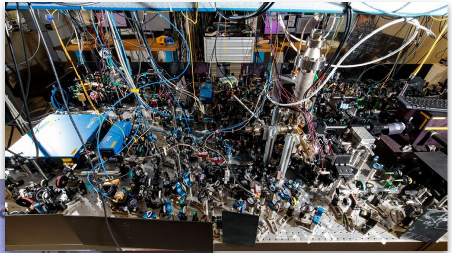


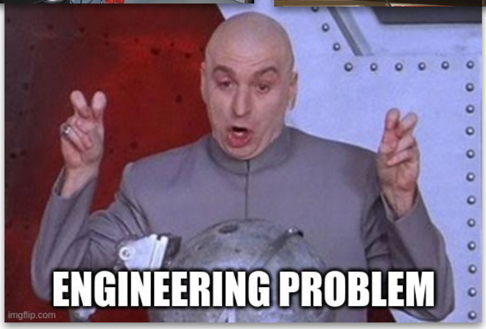
Turing Completeness doesn't always equate with practicality!

Why should I care?

- Engineering relies more and more on complex modeling and simulation tasks.
    - Trillions of elements
    - Tightly-coupled multiphysics
    - Uncertainty quantification
- We cannot accept black boxes in real engineering work.
    - If you don’t understand what you did, how do you know it is safe & reliable?
    - Can a future engineer understand what you did in your analysis long after you’re gone?
- We need people to build the future.
    - The quantum technology industry is new, but rapidly maturing.
    - In many cases, the physics is done, and everything is “just an engineering problem.”
    - Developing new products and applications requires different perspectives and skills.
- Quantum computing and technologies touch all of these.







Will it work?

- Today’s best quantum computers are prototypes.
  - “Noisy Intermediate-Scale Quantum” (NISQ)
  - <1000 qubits, error rates 10^{-2}-10^{-4}
  - Error correction, memory, and networking are needed
- No problems of large economic significance are being solved (yet).
  - Some niche exceptions with quantum annealing (D-Wave)
  - QPUs are too small and noisy
  - Very early demonstrations of error correction are happening now
- Problems of scientific significance will likely be first.
  - Benchmark problems
  - Physics, chemistry, materials science
- Valuable for research and education today!

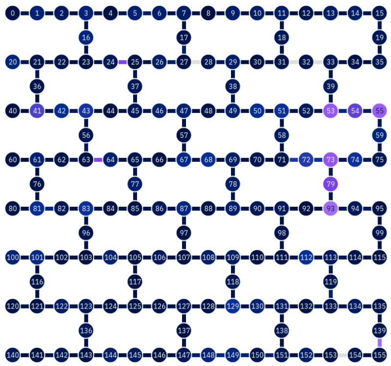
Where are we going?

Course Roadmap

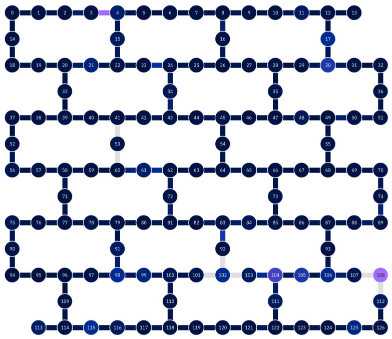
- Part 1 - Getting to Know the Hardware
  - Qubits, gates, and circuits
  - Hardware modalities
  - Qubit & machine characterization
  - Calibration & benchmarking
- Part 2 - Applications
  - Quantum Algorithms
  - Simulations
  - AI/ML
  - Optimization
  - Quantum Sensing & Networking
  - Supporting technologies (cryogenics, lasers, RF, …)

Our Hardware

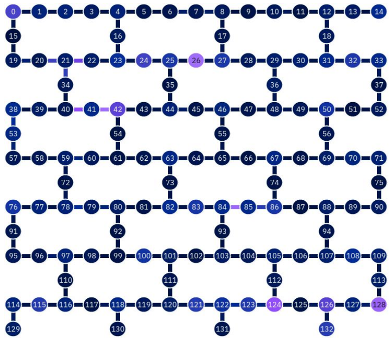
- IBM System One (VCC)
  - Superconducting transmon qubits
  - 127Q Eagle architecture
  - Fast turnaround (<1 minute)
- IBM Cloud Systems
  - 127Q Eagle - same as on campus, but different error profiles
  - 133Q and 156Q Heron architecture (5-10x lower error)
  - Need to wait in a job queue (seconds to days, depending on traffic)
- Simulators (your PC)
  - Simulate perfect qubits
  - Test noise models
  - <30ish qubits due to exponential scaling



IBM Fez (Heron v2)



IBM Rensselaer (Eagle)



IBM Torino (Heron v1)

Our Software

- Python (3.9 or later)
  - “The second best language for everything!”
  - I prefer Anaconda - better consistency between OS platforms.
  - We will use virtual (conda) environments.
- Qiskit
  - IBM’s quantum software development kit (SDK)
  - Supported on other quantum platforms (IonQ, Quera, Quantinuum, Atom Computing, …)
- Jupyter Notebooks/Jupyterlab
  - Web browser interface
  - Runnable “cells” of code interleaved with text, images, and math
- Optional Tools
  - Git - Version control, saves the full configuration state of your work (strongly recommended)
  - LaTeX - Document preparation and typesetting (great for beautiful technical documents)
- Other quantum SDKs and libraries (Classiq, Cirq, Q#, …) can be used for bonus assignments and Project 2.

Notation

- Quantum notation can be unfamiliar.
  - Dirac or “bra-ket” notation
  - Used mainly by historical accident
- The mathematical objects are familiar.
  - Scalars
  - Vectors
  - Matrices
  - Complex numbers
- The mathematical operations are linear algebra.

$$\boxed{|0\rangle} = \boxed{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}$$

The thing in the ket is just a label.
The thing it represents is just a vector.

$$|\psi\rangle = \boxed{\alpha}|0\rangle + \boxed{\beta}|1\rangle$$

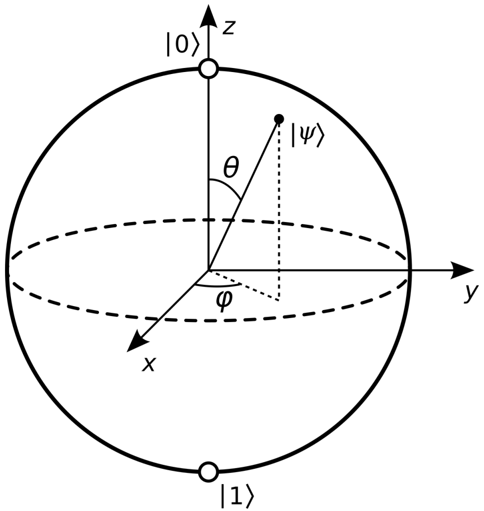
The coefficients represent how much of each qubit state is in the superposition.

$$|\alpha^2 + \beta^2| = 1$$

Quantum states are always normalized

Terminology

- Qubit - A quantum bit
- Gate - A single computational instruction that operates on one or more qubits.
- Circuit - A quantum program, consisting of gates acting on qubits
- State (or statevector) - The combined superposition of qubits before being read out.
- Noise - Physical effects that disrupt a qubit's state



The Bloch sphere plots the statevector of a single qubit.

More Terminology

- Basis States - The classical states of qubits (or groups of qubits) we use to create superpositions.
- Superposition - A quantum “mixture” of basis states that we get by applying gates.
- Probability Amplitudes - The coefficients in front of the basis states.
- Measurement/Readout - An action that draws a sample from the probability amplitudes, yielding a basis state state and disrupting the superposition.

Next Time

- Basics of qubits:
  - Review of terminology, math, and notation
  - Translating math to code (and back)
  - Measures of qubit quality
- Playing with qubits:
  - Gates, states, and operations
  - Simulation vs. Reality
  - Characterizing qubits - coherence time and fidelity
- Hardware implementations:
  - Design requirements for qubits
  - How qubits are physically made and programmed
  - What happens when you run a program

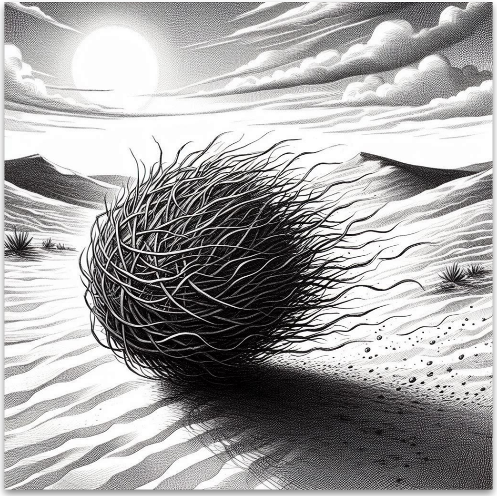
Homework 1

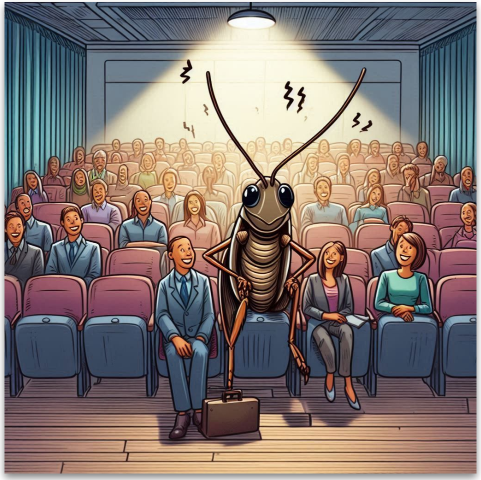
- Environment Setup
  - Install Anaconda/Miniconda
  - Create IBM Accounts.
  - Register machine access.
- Run simple programs
  - “Smoke test” to make sure everything is working
  - Steps 1-4 of the Qiskit “Hello World” example.
  - Bonus idea: Do the remaining steps of the tutorial.
- Reading & Free Response:
  - Read the McKinsey 2024 Quantum Technology Monitor.
  - Answer 3 open-ended questions, no right or wrong answers.

Resources

- RPI DotCIO QED Office Hours - Wednesdays
- IBM Quantum Office Hours - By Announcement
- Qiskit Youtube Channel - https://www.youtube.com/Qiskit
- Quantum Computing for the Curious - https://quantum.country
- More to come on LMS!

Questions & Discussion





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2. R. P. Feynman, *Quantum Mechanical Computers*, Found Phys **16**, 507 (1986).
3. P. W. Shor, *Algorithms for Quantum Computation: Discrete Logarithms and Factoring*, in *Proceedings 35th Annual Symposium on Foundations of Computer Science* (1994), pp. 124–134.