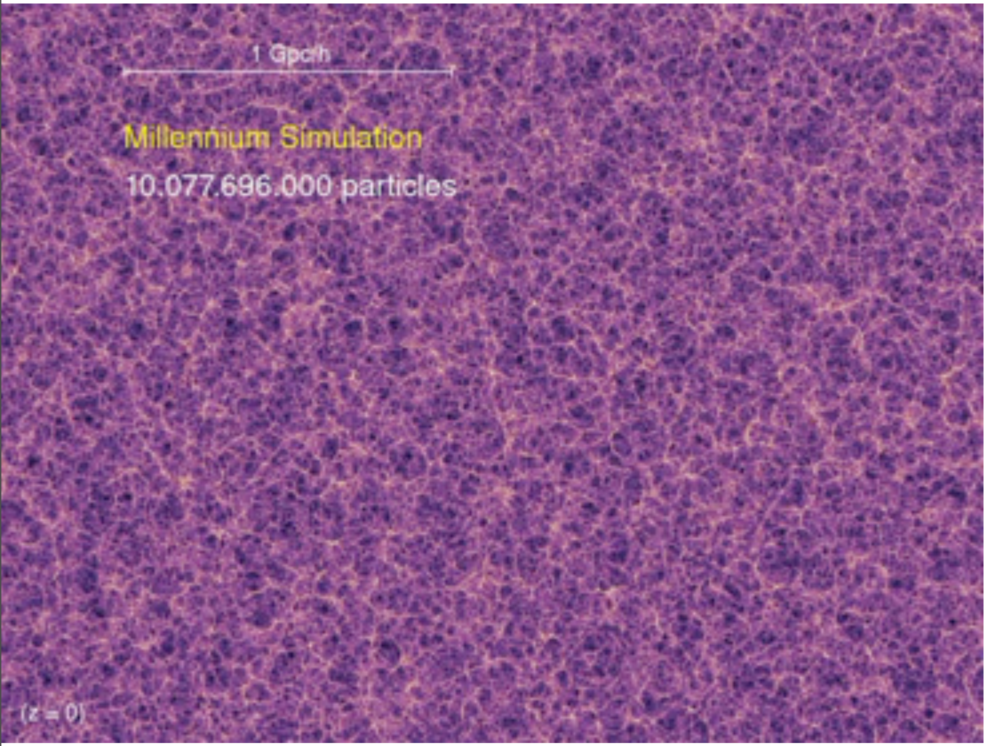
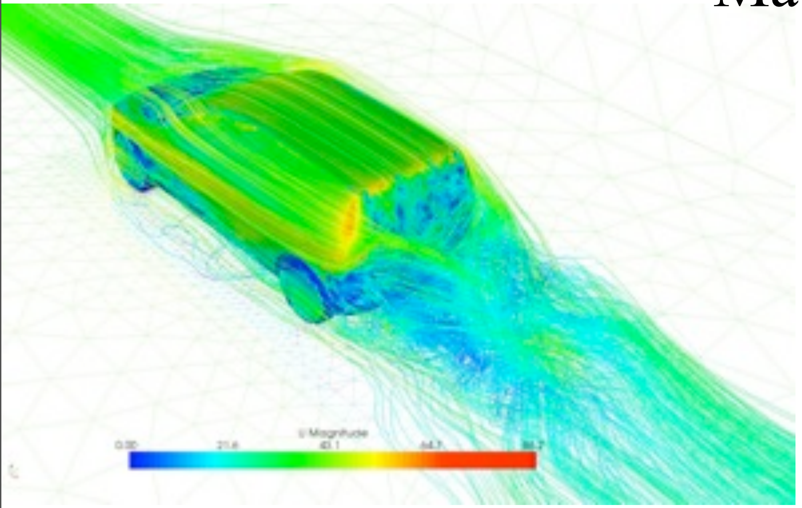
What do Climate Modeling and Quantum Mechanics have in common?

Chaos, Quantum Mechanics, and Computers



Dark
Matter

Computer simulation: now one of the most important ingredients for progress...



Quantum
spins

Technology and Engineering

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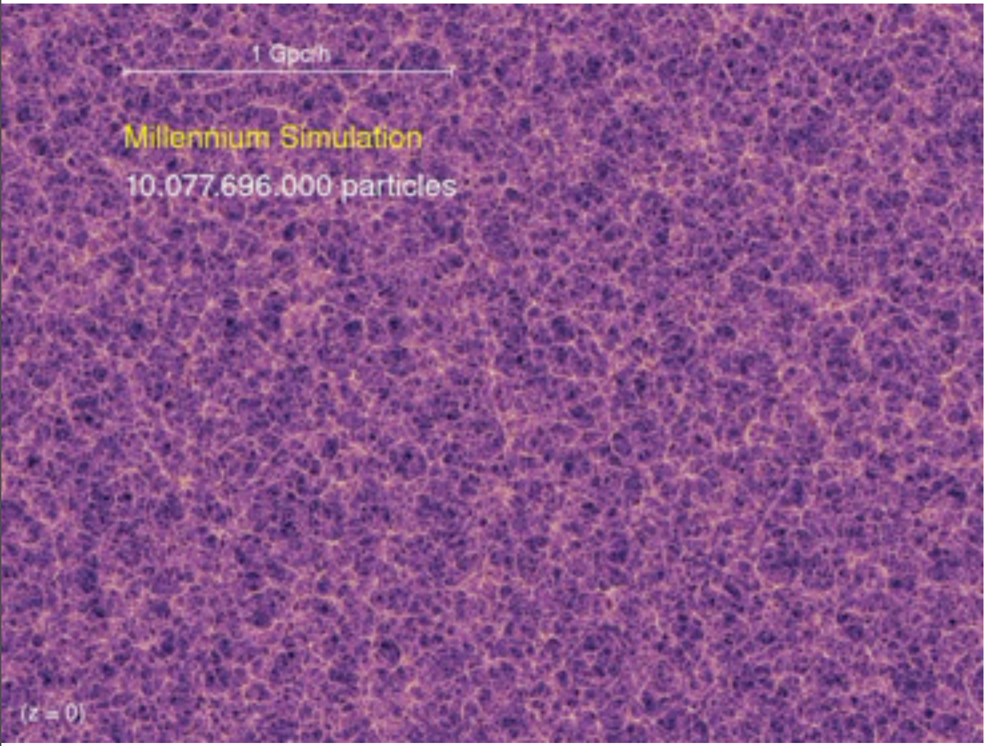

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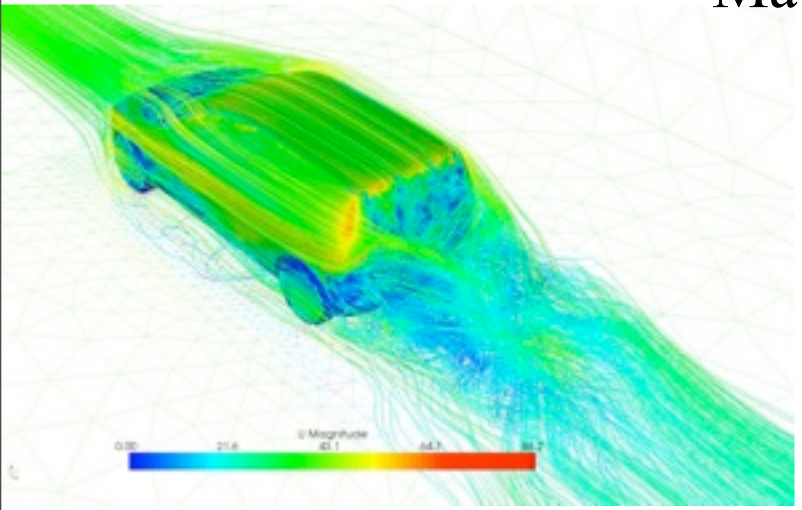
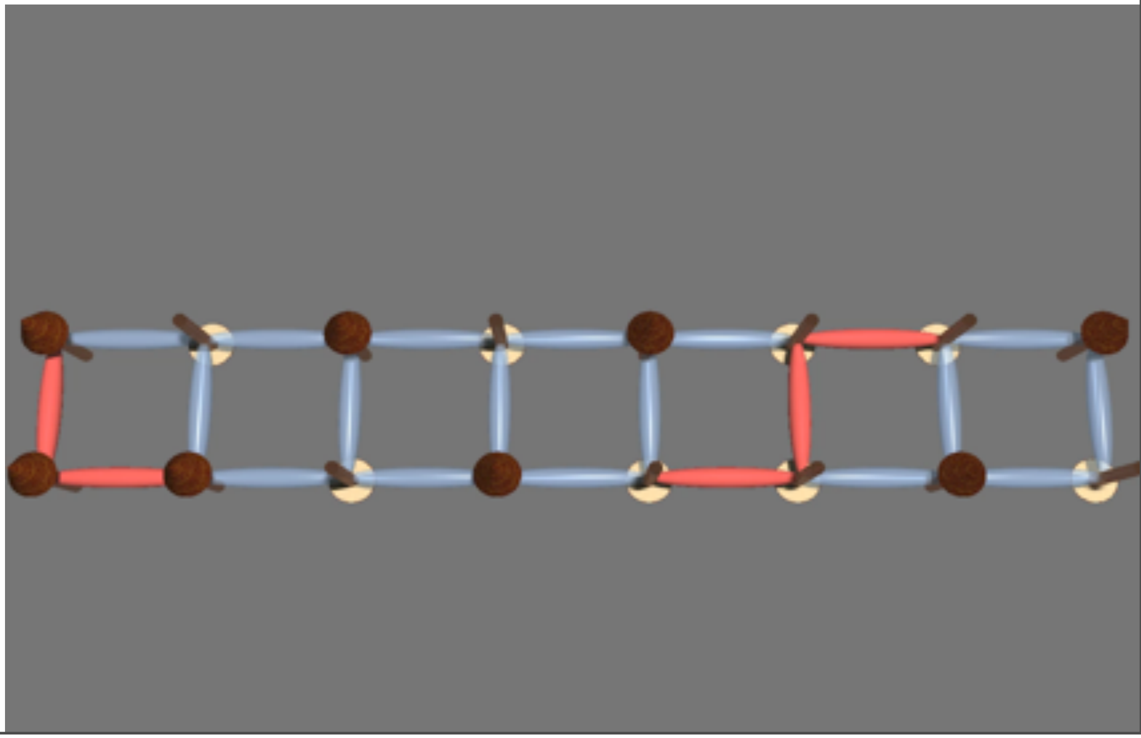
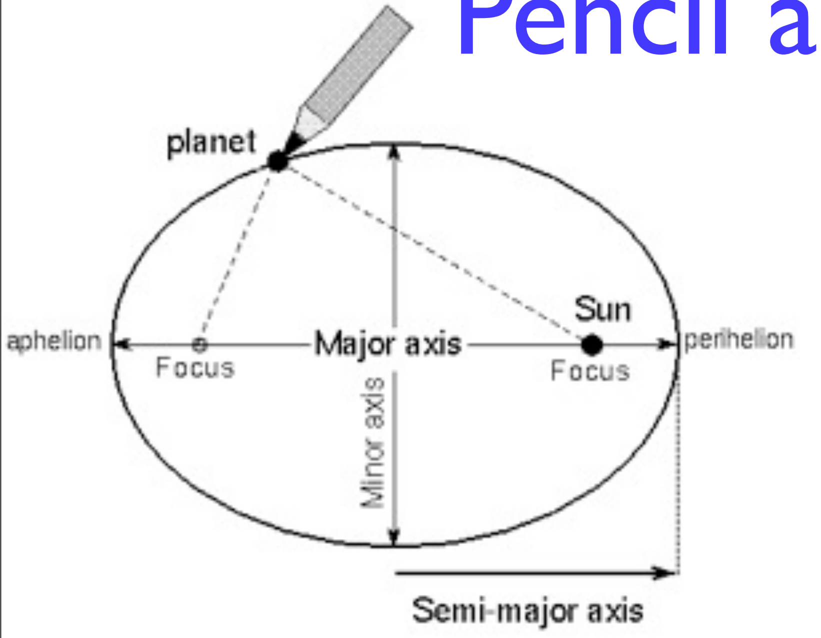


Technology and Engineering

Quantum spins



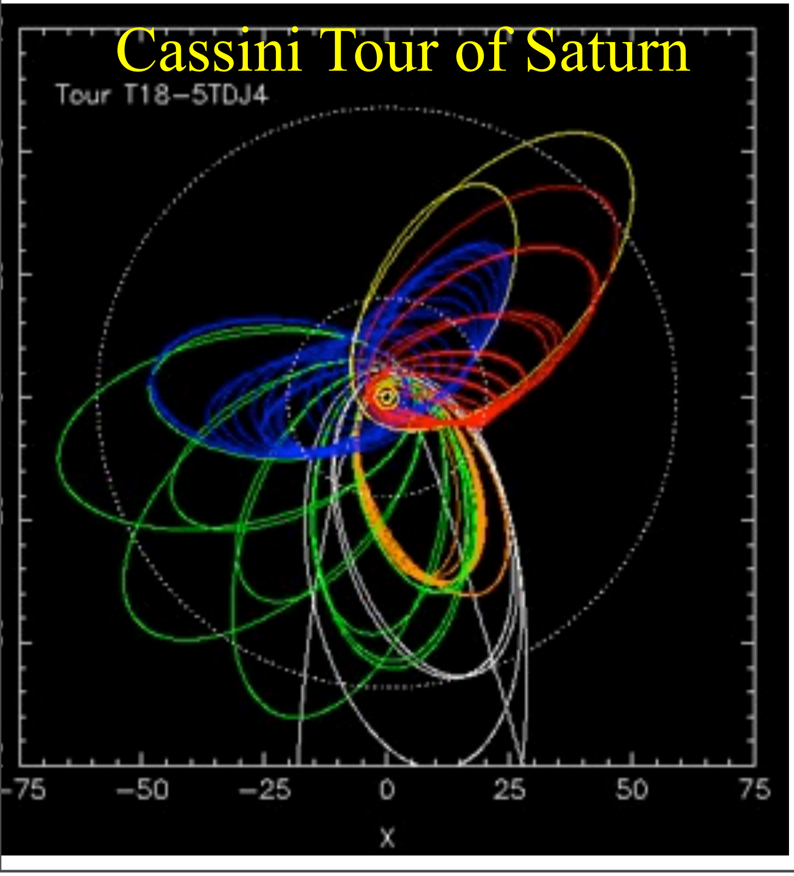
Pencil and Paper, or a computer?



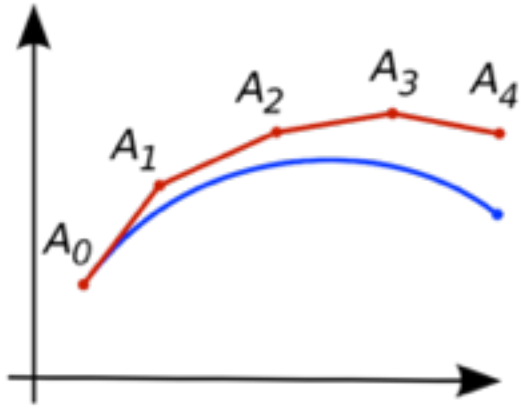
- Planetary motion: Isaac Newton used pencil and paper to prove Kepler's first law and derive planetary motion! (Before that, he *invented* classical mechanics!)

"If I have seen further it is only by standing on the shoulders of giants."

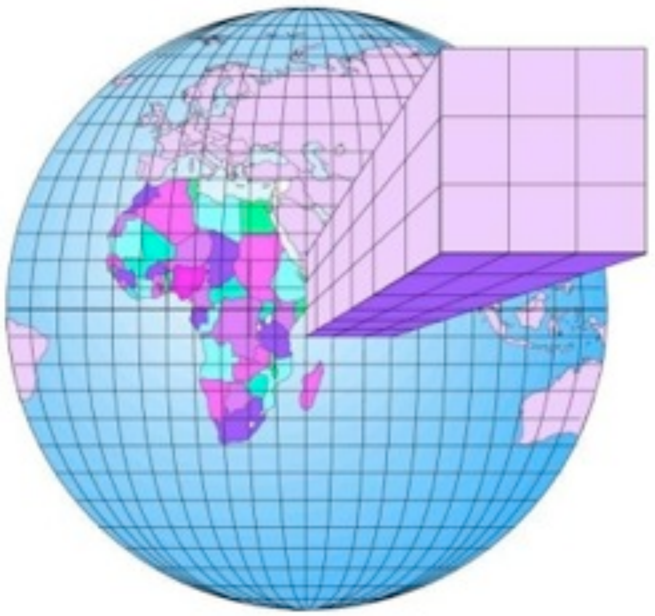
- Three or more objects: analytic approach becomes almost impossible.
- To solve the hard problems on a computer, break up the problem into lots of little, simple pieces.
- The solutions to the little pieces are easy and the computer can use them very quickly


Cassini Tour of Saturn

The standard computational approach to physics: break the problem into little pieces



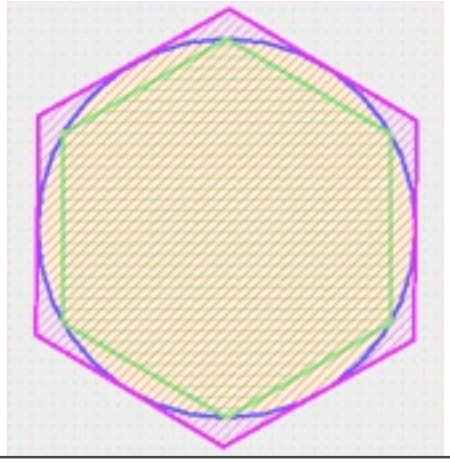
Particle motion: go in a straight line for a short time, then recalculate the direction and speed. The shorter the time intervals, the greater the accuracy.



For weather and climate modeling, assume the temperature, pressure, wind velocity, etc are approximately constant over a “little” cube. The smaller the cubes, the greater the accuracy.

This approach goes all the way back to Archimedes(!) who used it to approximate π. Result for a 96-gon:

$$223/71 < \pi < 22/7$$



Progressing from just *hard* to *impossible*!

Hard: simulating detailed planetary motion for more than 1 billion years!

Poincaré: Consider just three planets, but with no sun and equal masses: ***Chaos***

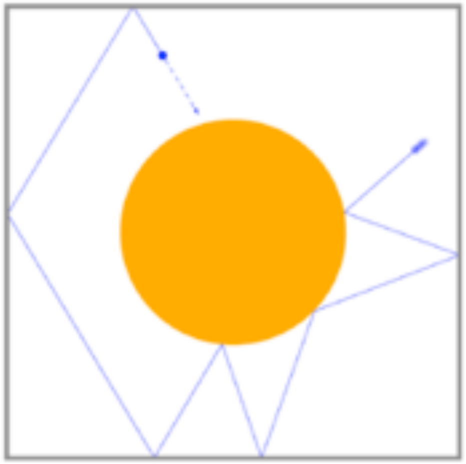
Poincaré
1854-1912

The key feature of chaotic systems: very very tiny differences in how you start the system give huge differences in the results: the errors grow *exponentially* with the time.

Impossible: simulating a chaotic system accurately for a long time

A simpler example due to Sinai is “Sinai billiards”

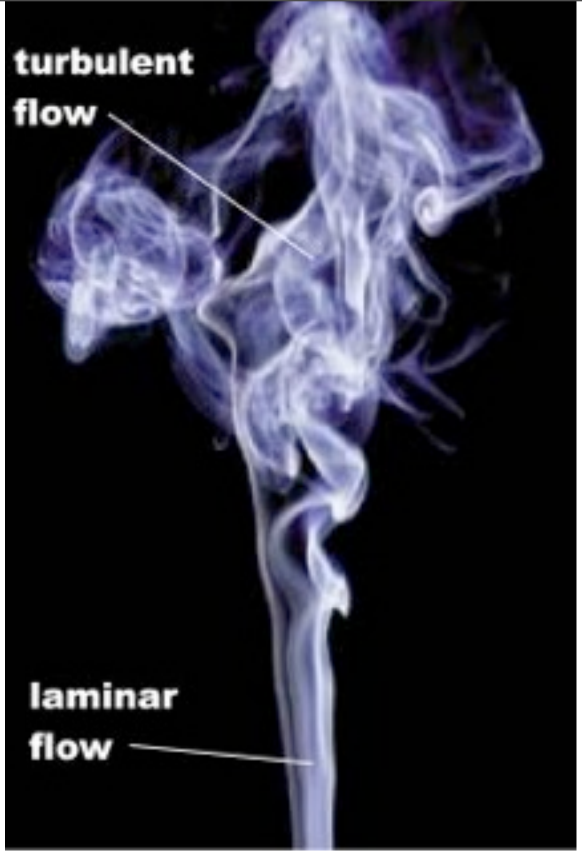
Ordinary billiards also exhibits chaos, which might be useful in “pool hustling”



Sinai Billiards


STA Travel
Wells Fargo Bank
SchoolsFirst FCU

Chaos and the weather



Some of the very first computer simulations of the weather by Lorenz showed chaos, which is tied to turbulence.

The “butterfly effect” is from a talk given by Lorenz to the AAAS in 1972: “*Predictability: Does the Flap of a Butterfly’s Wings in Brazil set off a Tornado in Texas?”*

The basic “time-scale” for weather prediction is about a week. With a big computer we may do OK for two weeks, but two months is hopeless and always will be!

Then how can we predict climate change?

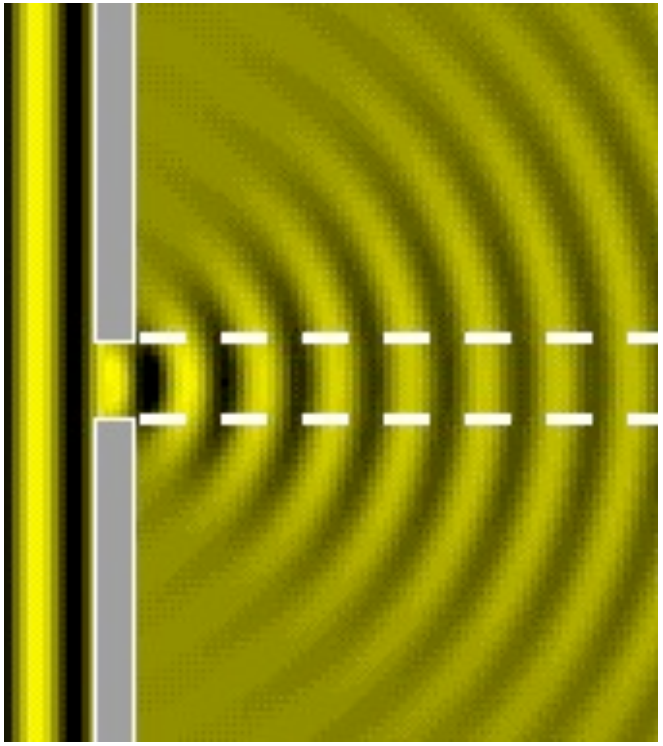
Quantum Mechanics

- Classical Mechanics is an extremely good approximation in every day world
- But it fails for tiny objects--atoms, electrons, photons (particles of light)
- *Are particles really particles, or are they waves?*
- Sometimes quantum mechanics has effects on the macro-scale!

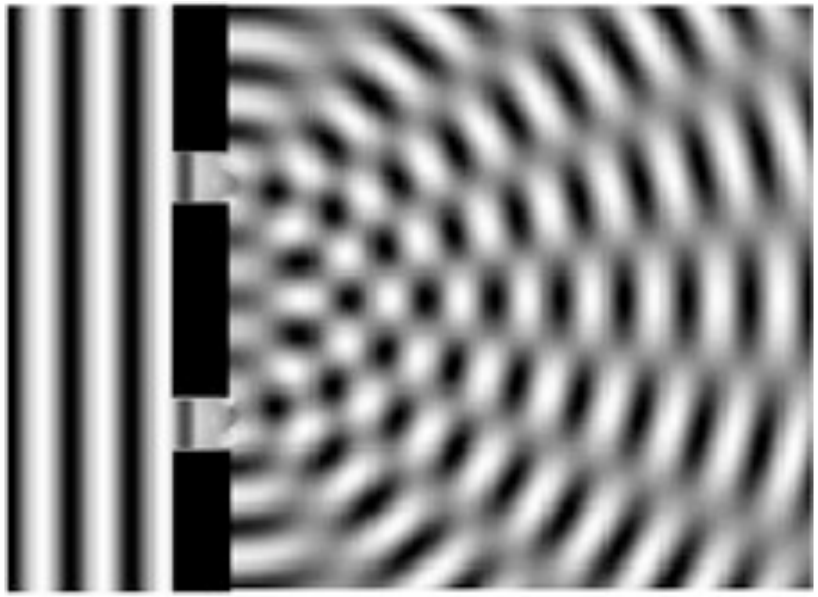
Water waves

The first step in understanding quantum mechanics is understanding the difference between waves and particles.

Waves from pebbles in a pond

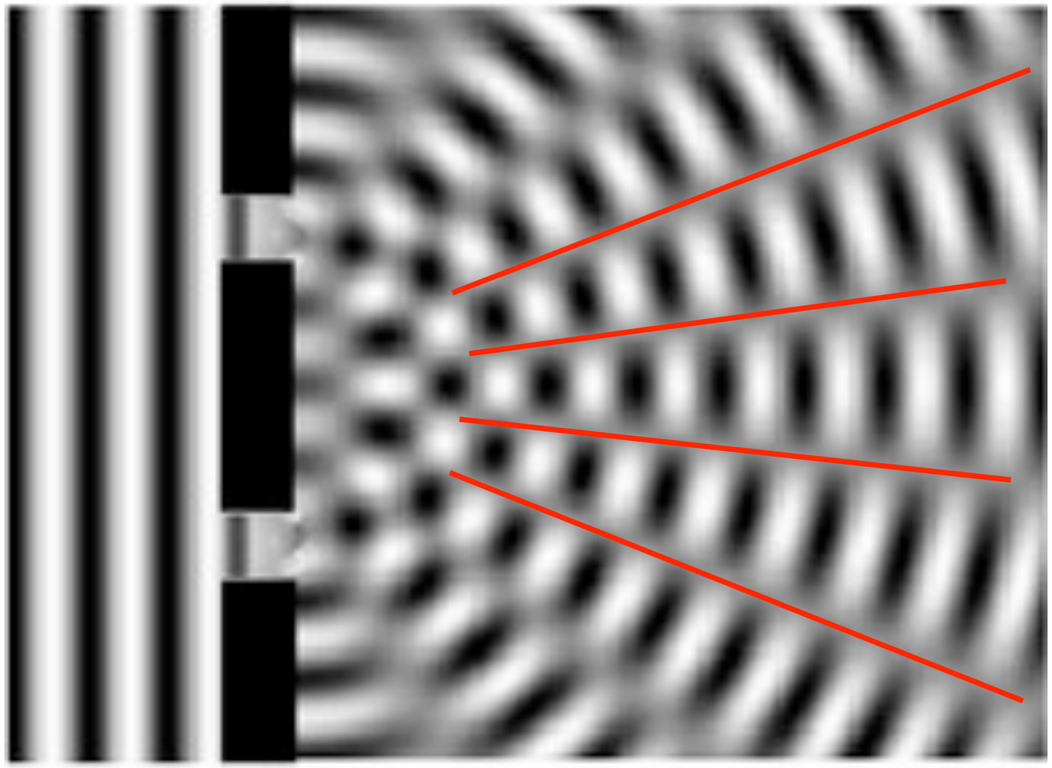


Straight waves hitting a single small slit make circular waves

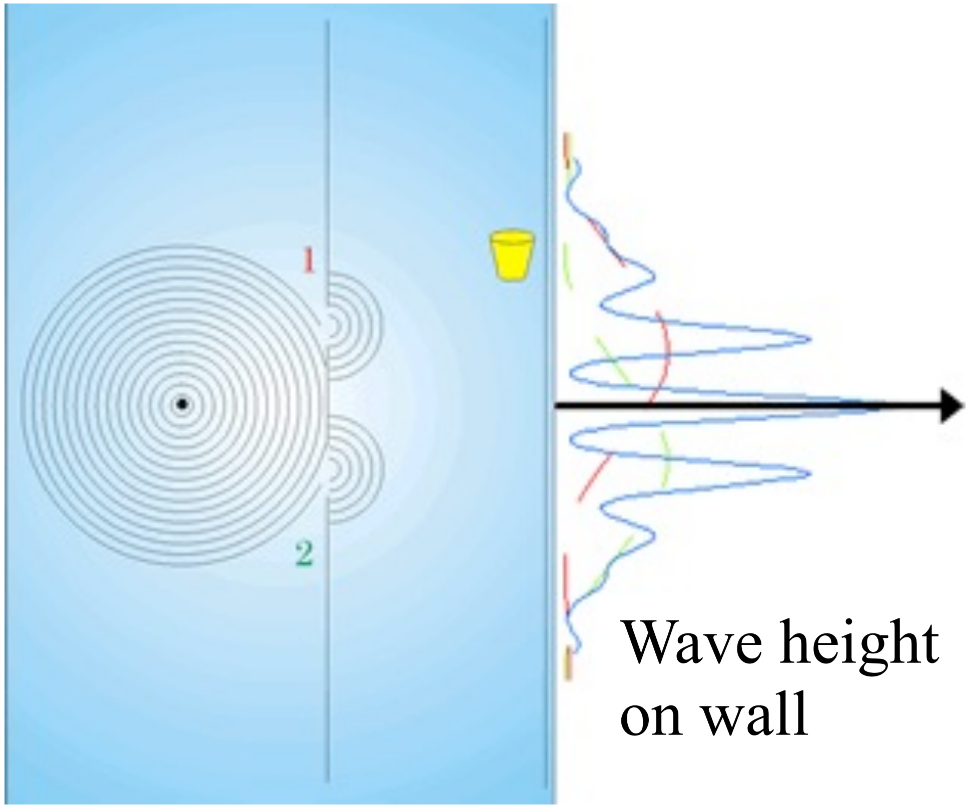


Waves hitting two slits: interference

Interference patterns

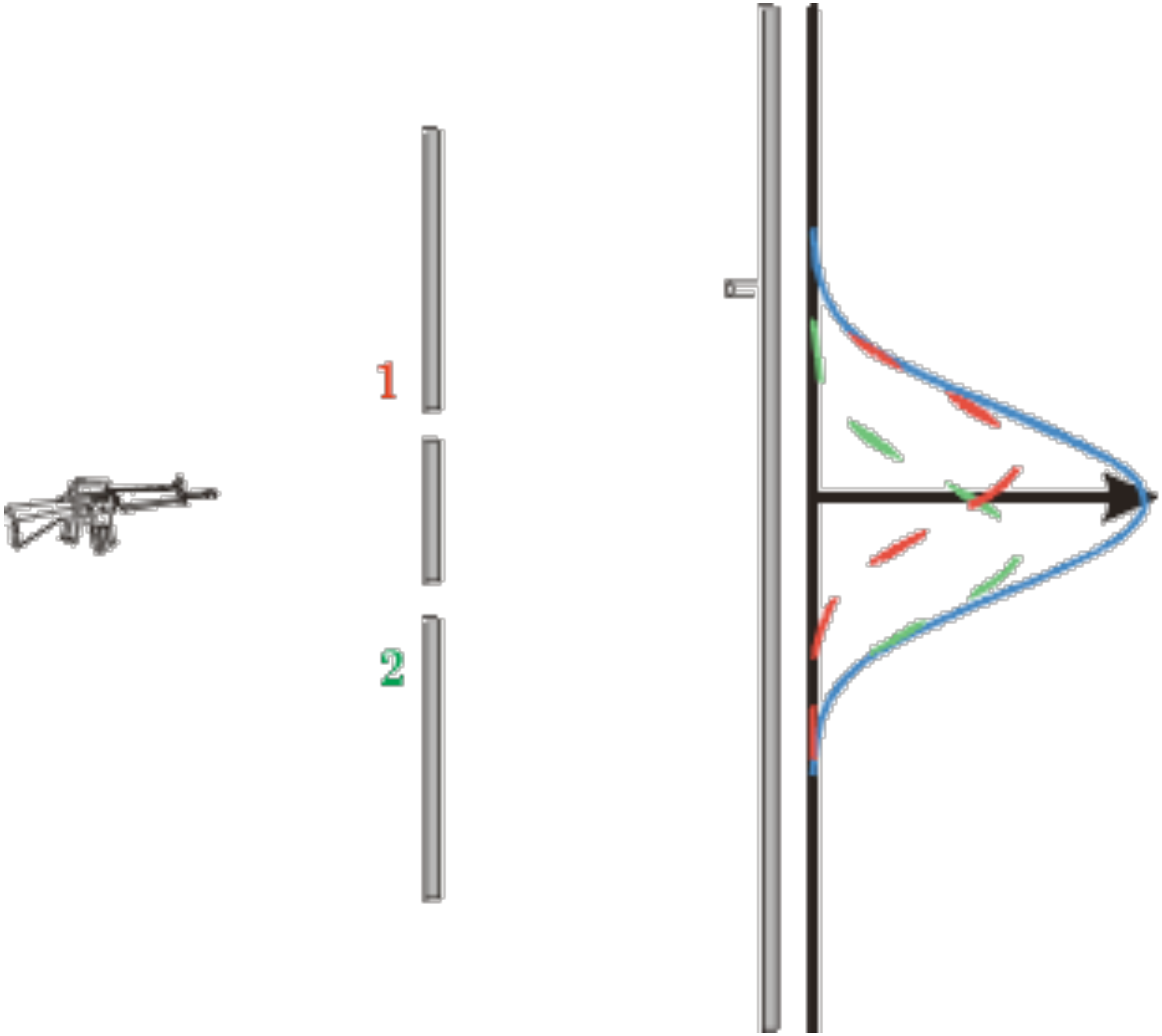


Red lines show where waves cancel

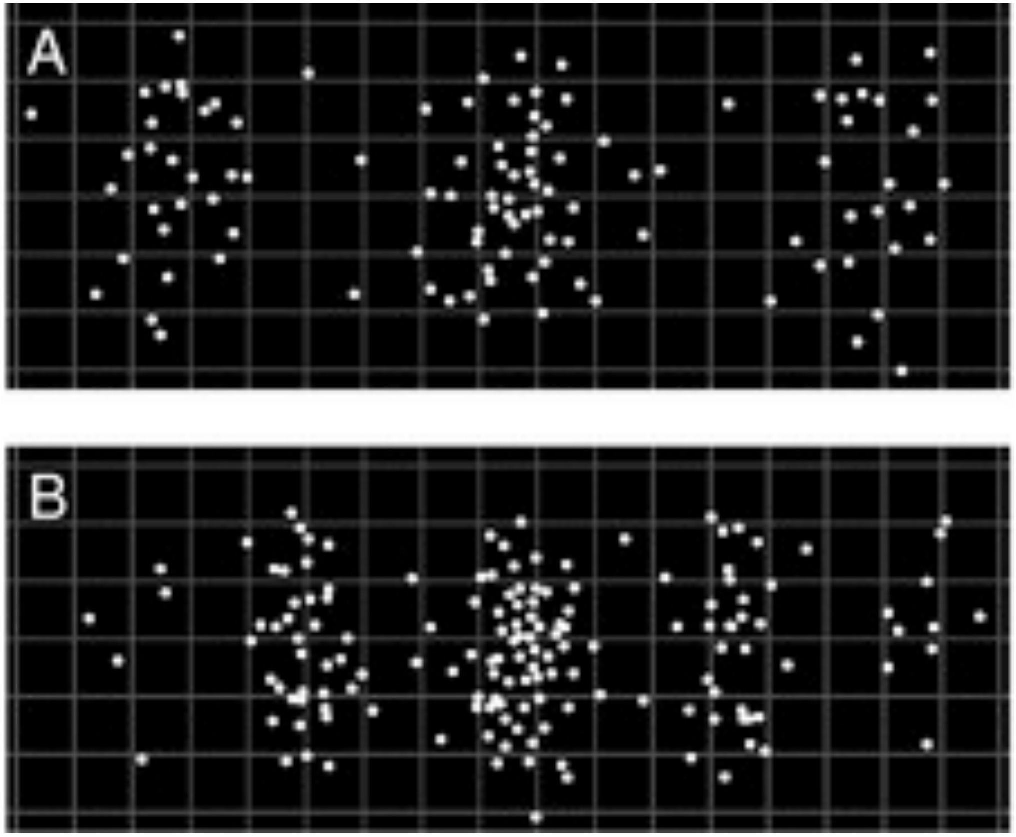


Wave height on wall

Particles (like bullets) don't have interference patterns



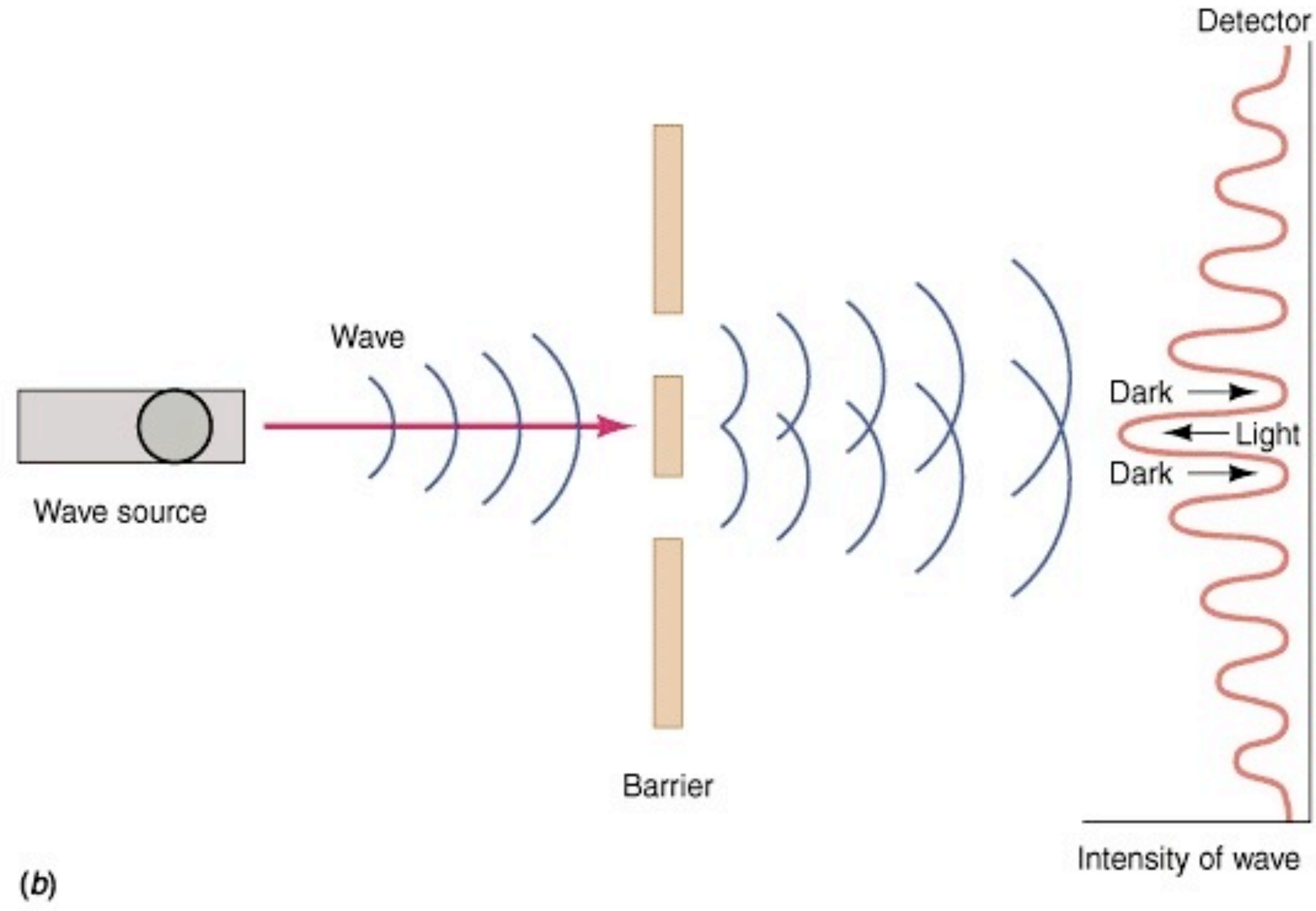
What do electrons do?



Is the pattern from two electrons interfering with each other? No, it happens even if the electrons go through one at a time!

Why do electrons interfere?

- A quantum particle is described by a "wavefunction"--it acts like a wave until you look at it.

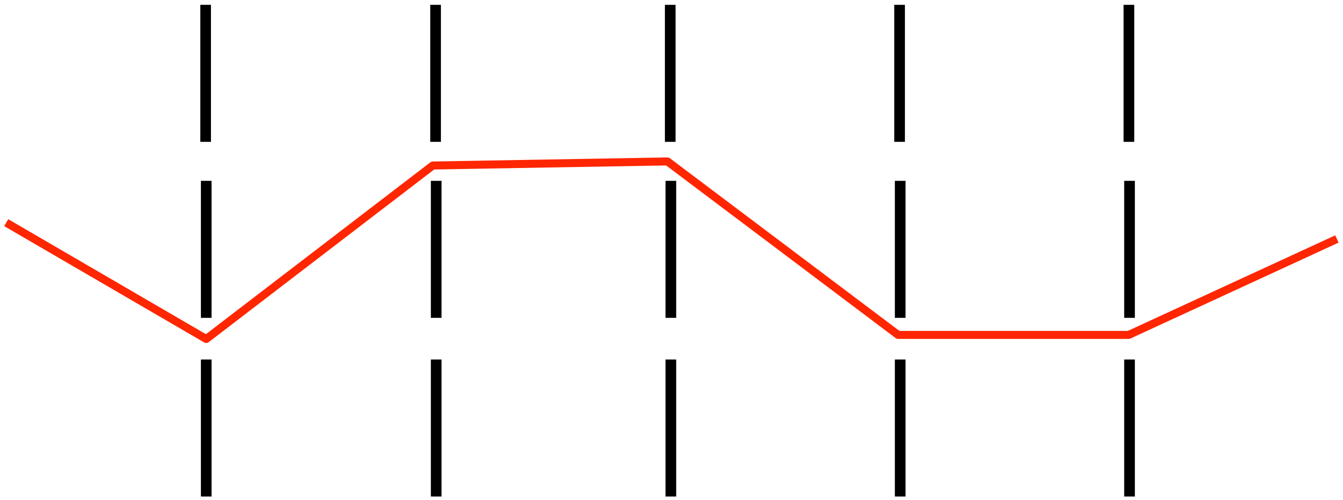


Which slit did the electron go through?

- This sort of question has puzzled physicists for 80 years!
- Suppose you try to look at a slit (shine photons at it). You find out which slit it went through but you also destroy the pattern!
- Here is one way to answer the question: “The wavefunction goes through both slits.” But is the particle the same as its wavefunction? Is the wavefunction real?
- Feynman: “no one understands quantum mechanics”

Simulating quantum mechanics on a computer

- Two key strange principles for simulating QM:
  1. Some things absolutely cannot be predicted except as a probability. (If you look to see which slit it went through, was it the top or the bottom? 50-50) But QM predicts precise results for *statistical averages*.
  2. When you are not "looking", everything that could happen, does happen! Every possibility combines together to give the final answers.



One possible path out of 2^N total!

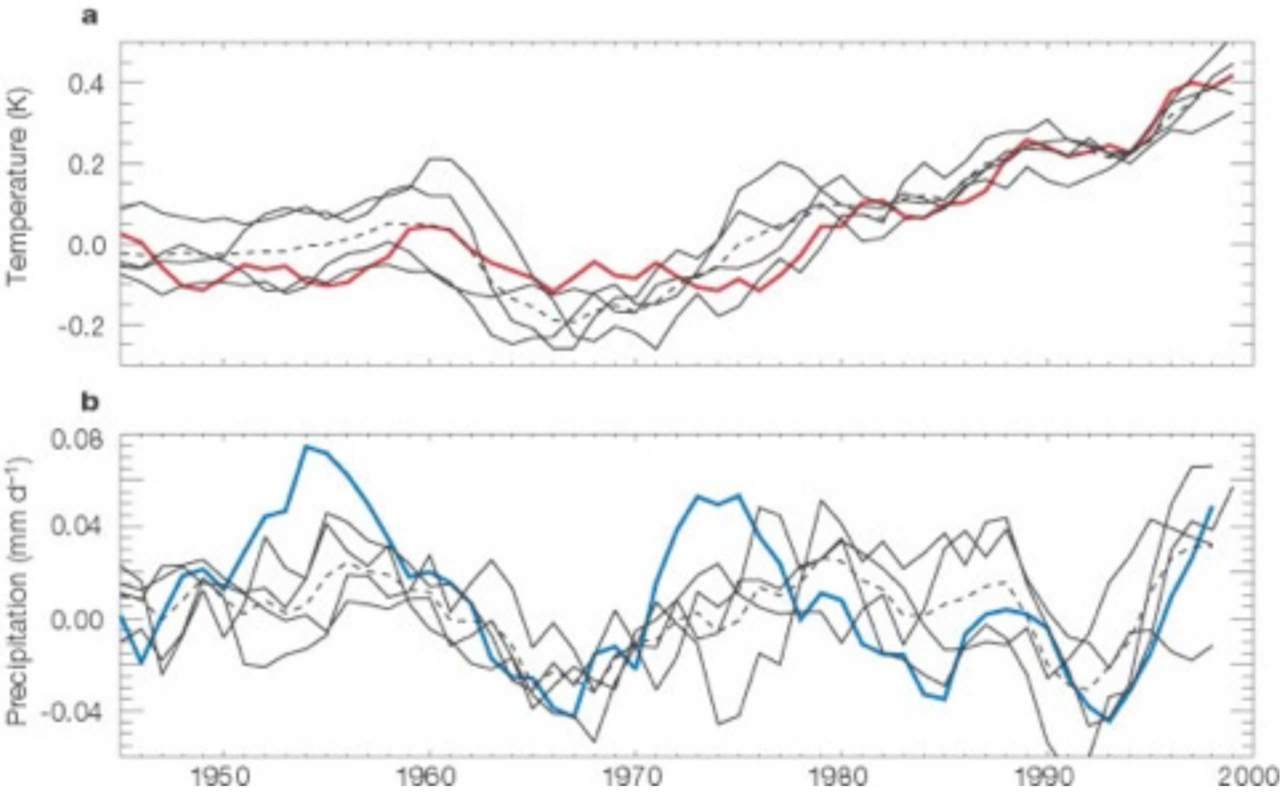
Simulating quantum mechanics is exponentially hard!

Simulating chaos and quantum mechanics: surprising similarities

- Some questions we would like to answer cannot be answered: Which slit? Will it rain next Christmas?
- The questions we can answer are often about averages and probabilities. (What will the world-wide average July temperature be next year?)
- Einstein said "God does not throw dice". Einstein didn't like the randomness appearing in quantum mechanics. But one of the best ways of dealing with chaos and quantum mechanics on the computer is to "roll the dice".

Simulating climate

- How can we simulate climate for 500 years if we can't simulate the weather for a week?
  1. Look at averages over large areas and long times so the stuff we can't predict averages out.
  2. "Roll the dice" to do "ensembles" of simulations



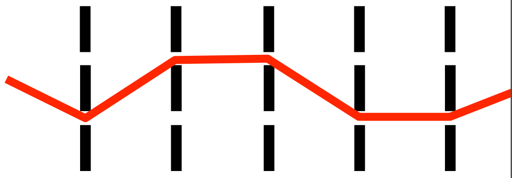
Colored lines: real-world measurments

Black lines: Four different simulations of the same thing, with slight random variations

This is from a 2002 Nature paper. Nowadays people do ensembles of more than 100.

Simulating quantum mechanics: quantum Monte Carlo

- How can we sum up the exponentially large number of paths?
- The answer is just like predicting an election with a poll. For an ideal prediction we would call every voter in the country. Instead, we roll the dice, and pick people at random. Calling about 1000 people works pretty well (ideally) and it wouldn't matter if the population was 1 trillion!
- In quantum Monte Carlo, we pick *paths* at random and add them up. If we do this cleverly and nature is kind, it works, we can get the answer for 10^{1000} paths by sampling a million...



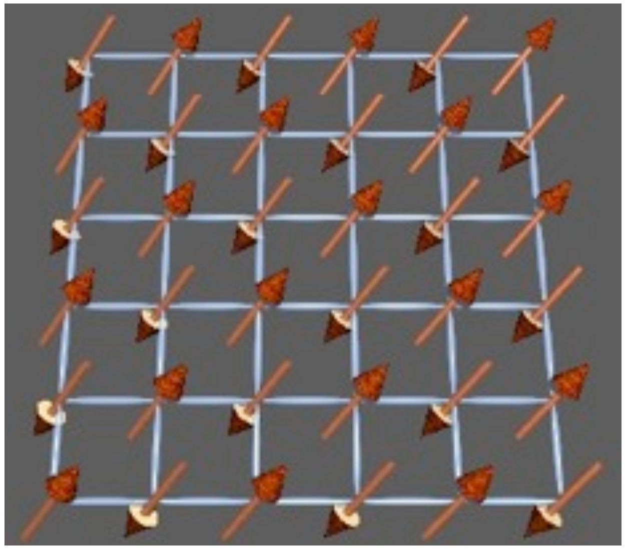
$+$

$\cdots$

quantum Las Vegas?

How important is quantum Monte Carlo?

- Ask google scholar: a search on "quantum Monte Carlo" produces 24,000 hits
  - Used to understand high temperature superconductivity, the quark structure of protons and neutrons (lattice gauge theory), spin liquids, molecules, etc.
- Ask google scholar: a search on just "Monte Carlo" produces about 2 million hits!
  - Every field of physics and almost all science uses Monte Carlo, even experimental areas

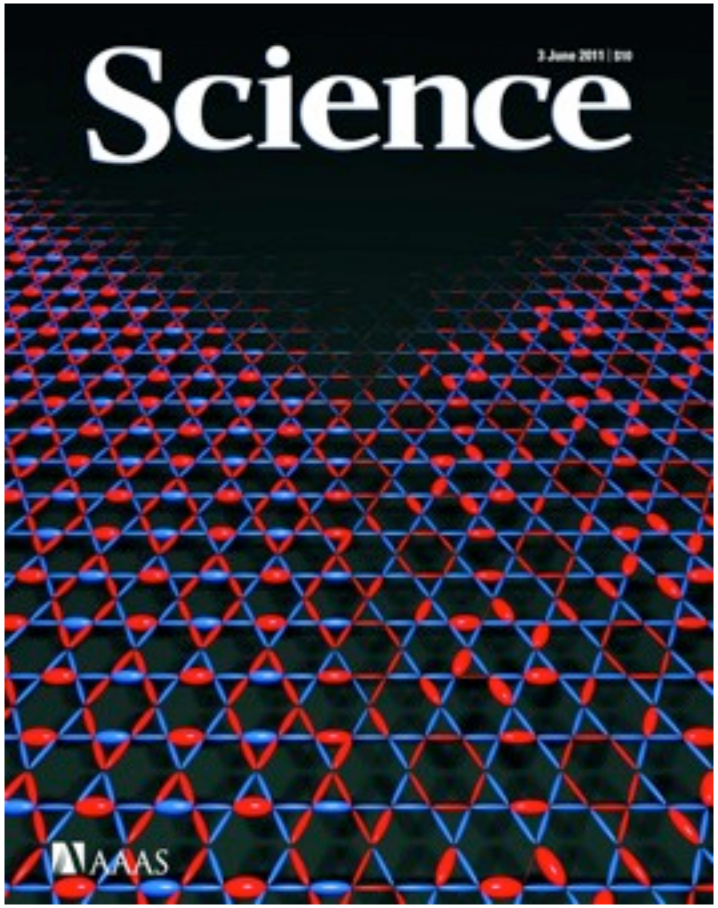


This is a real example of what we use "QMC" on: spin systems

This one describes the "parent compound" of a high temperature superconductor

Does quantum Monte Carlo always work?

- Alas, no. Sometimes nature gives us problems that are like an election that gets decided by a couple of votes... Overcoming this problem is one of the hottest areas of research...(and also *my* area!)
- The important problems in QM don't involve slits and electrons going through them. But systems of quantum *spins* are important and mathematically they resemble slits and electrons.



Quantum
spin
Liquids

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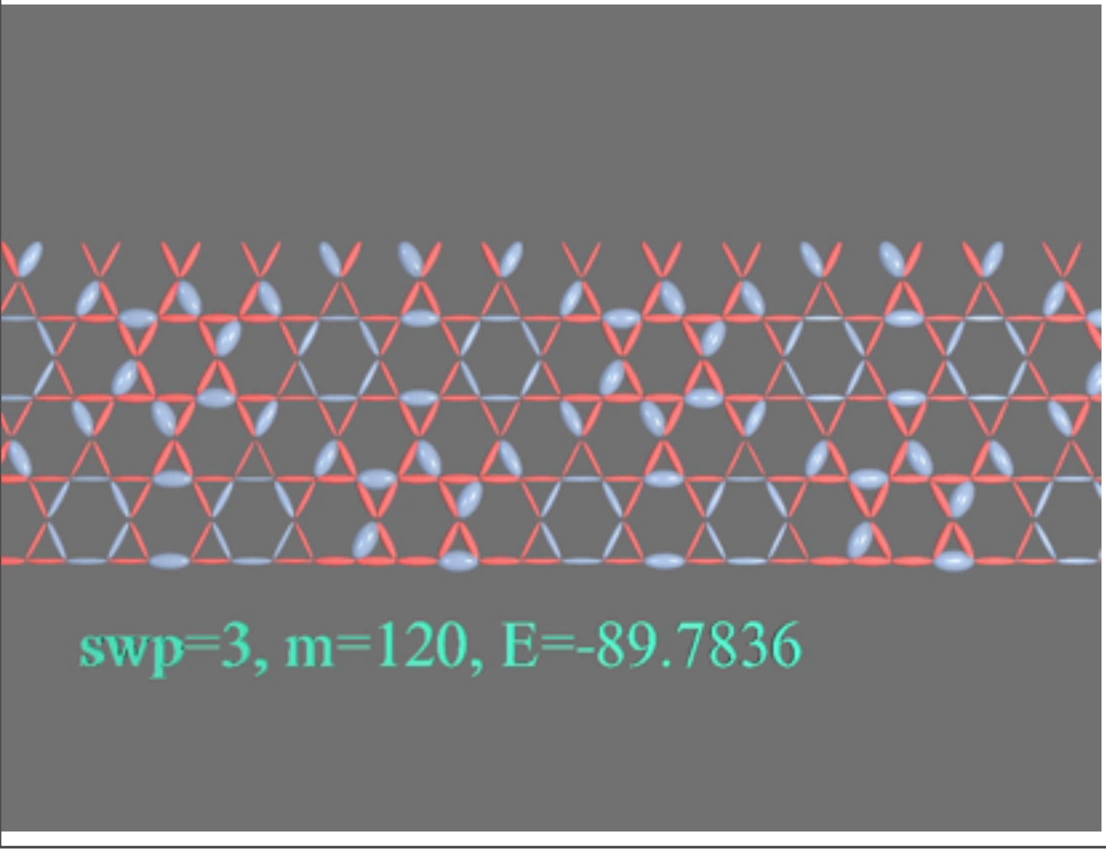
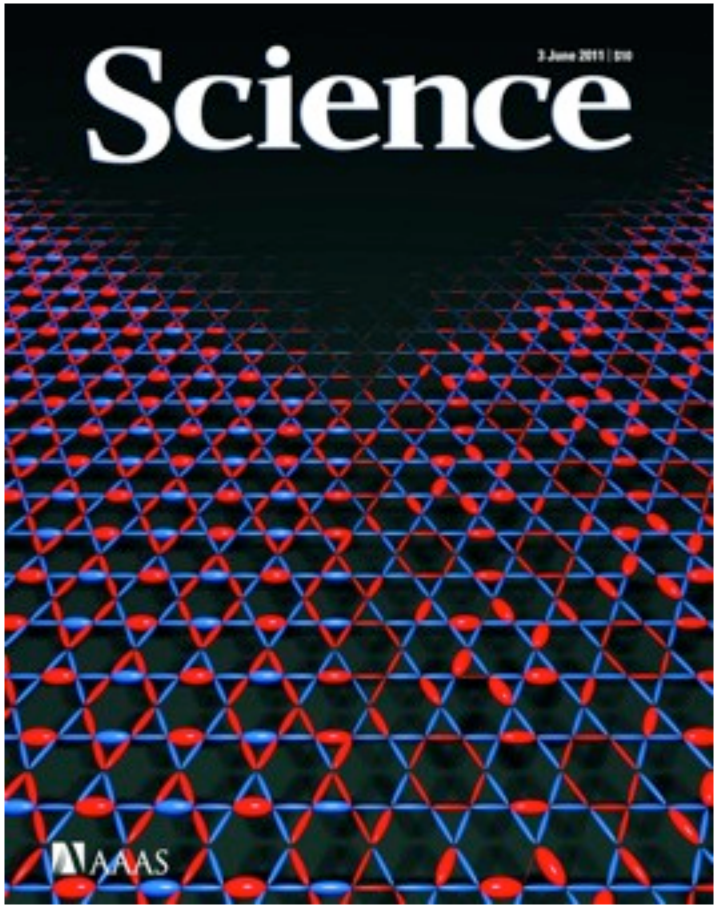


Quantum spin Liquids



Summary: simulating chaos and quantum mechanics

- For both chaos and quantum mechanics, some questions we would like to answer cannot be answered.
- The questions we can answer are often about <u>averages</u> and <u>probabilities</u>.
- For both chaos and quantum mechanics, we can get around the <u>exponential</u> difficulty by "rolling the dice", using randomness as an ally in our simulations: ensemble simulations and quantum Monte Carlo.
- The forefront of research in quantum simulations is what to do when quantum Monte Carlo doesn't work.

Thanks to:

The KITP

The National Science Foundation

and

Thank you for your attention!

Some delightful books for the general audience:

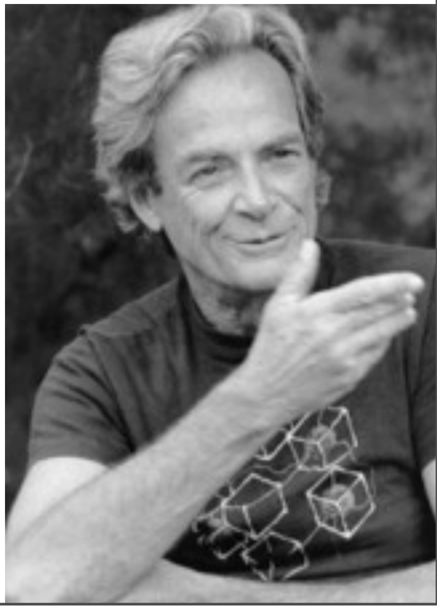
Six Easy Pieces by Richard Feynman

Chaos: Making a New Science by James Gleick

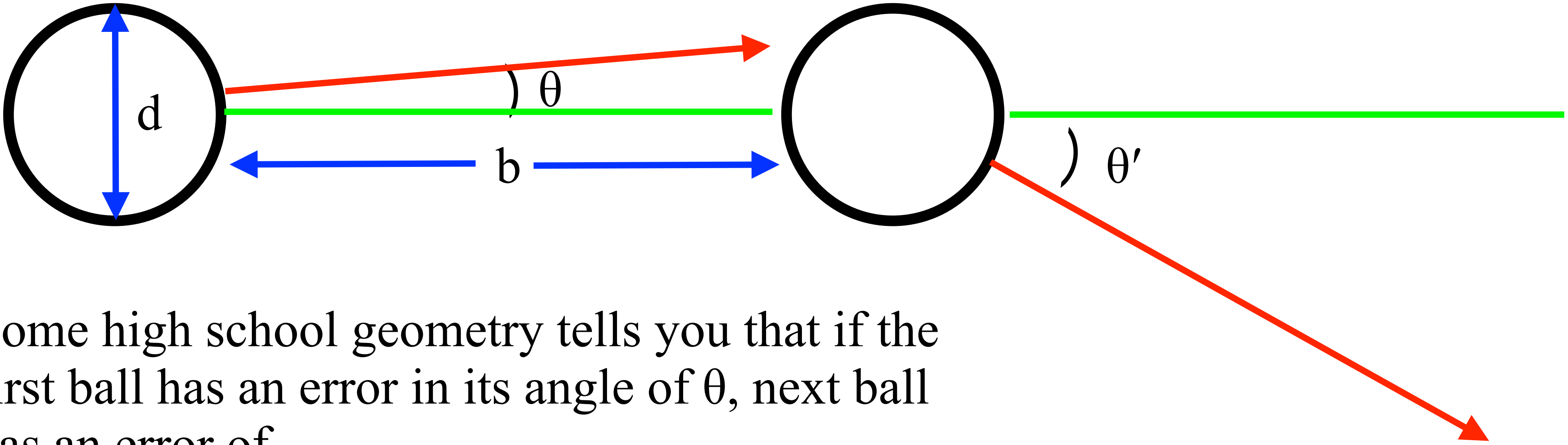
Simulating quantum mechanics: why is it so important?

- Understanding materials and predicting new ones:
  electronics, magnetism, superconductivity, "spintronics", ...
  (see MIT Professor Patrick Lee's talk in two weeks!)
- Understanding the "standard model" of particle physics ("lattice QCD")
- Understanding new states of matter (cold atomic gases, quantum Hall states...)
- Understanding chemistry:

"All these [chemical] rules were ultimately explained in principle by quantum mechanics, so that theoretical chemistry is in fact physics. On the other hand, it must be emphasized that this explanation is in principle. We have already discussed the difference between knowing the rules of the game of chess, and being able to play." --Richard Feynman



Billiard ball collisions



Some high school geometry tells you that if the first ball has an error in its angle of θ, next ball has an error of

$$\theta' = \theta \times \frac{b}{d} \qquad \text{if } \theta \text{ is small}$$

So, if the balls are 2 inches in diameter and 12 inches apart, each collision magnifies the error by a factor of 6.

$1/6° \rightarrow 1° \rightarrow 6° \rightarrow 36° \rightarrow$ miss   Exponential growth of the errors!