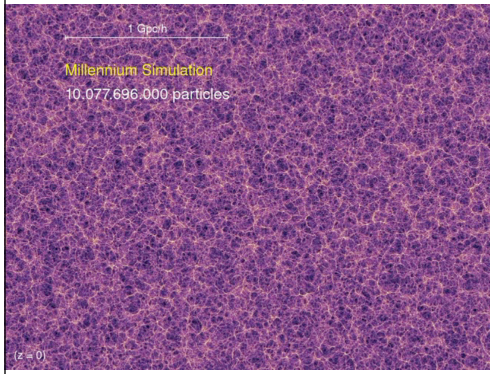
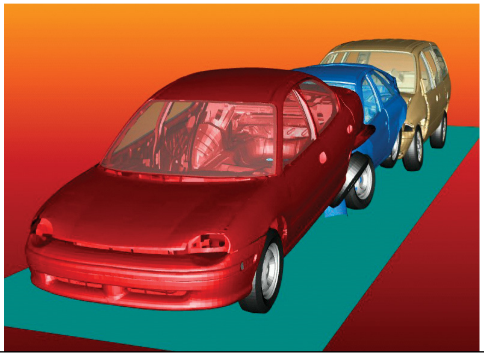
Chaos, Quantum Mechanics, and Computers



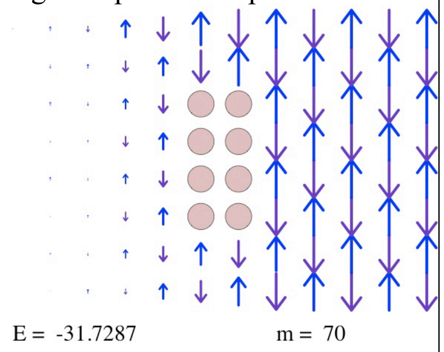
Computer simulation of the world around us is one of the most important ingredients for progress...

Dark Matter

Technology and Engineering



High temperature superconductors



Spins on an atomic lattice of copper and oxygen atoms forming “stripes”

Chaos, Quantum Mechanics, and Computers

Today many many systems can be simulated on a computer. The hardest ones to deal with are the ones with either *chaos* or *quantum mechanics*.

How do you make a computer simulate even an easy physical system?

What is chaos?

What is quantum mechanics?

How can we get around the exponential barriers to simulating systems with chaos or quantum mechanics?

"Computer Defeats Kasparov, Stunning the Chess Experts"

--NY Times, May 5, 1997

How did Deep Blue beat the world champion?

- Kasparov
  - Genius level understanding of strategy and tactics
  - Huge knowledge of historical games and patterns
  - Brilliant (for a human) ability to think through hundreds of moves quickly

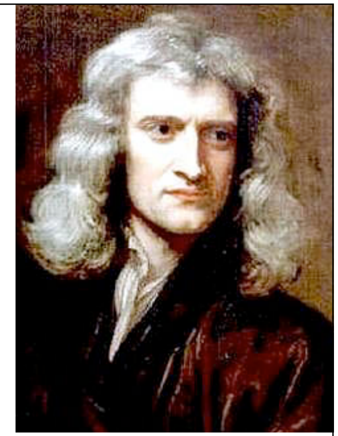
- Deep Blue
  - Basic evaluation of who is winning in any position
  - *200 million positions per second*
  - Clever pruning of irrelevant branches of the possible-move tree

People vs Computers

- Humans solve hard problems using intuition, knowledge, deep understanding, advanced math...
- Computers can solve many hard problems by breaking them into many simple parts and processing them extremely rapidly
- Clever *algorithms* can make all the difference in whether the computer can solve the problem

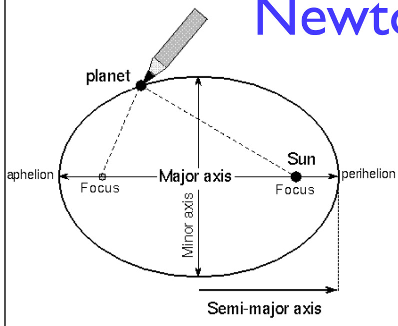
Isaac Newton (1643-1726)

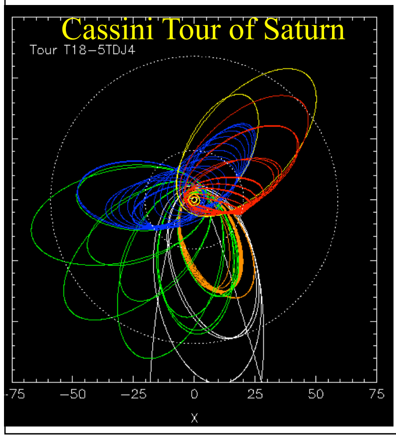
- Often called the greatest scientist of all time
- "Invented" calculus, optics, mechanics (Newton's law of motion), the theory of gravitation, planetary motion, the reflecting telescope...
- Also obsessed with alchemy and suffered massive mercury poisoning. In later years he became quite eccentric... Derived from the bible that the world won't end before 2060...
- Newton's creation is called *Classical Mechanics*. Classical mechanics does a marvelous job of describing everything but the very smallest and very largest objects. But--you have to solve the equations!



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

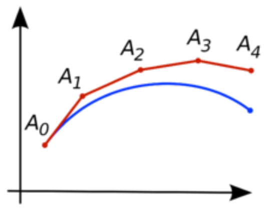
Newton and Planetary Motion



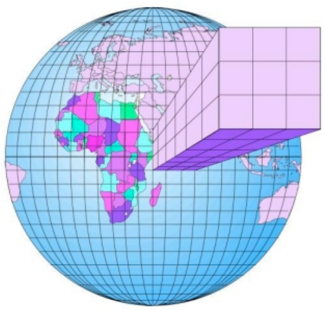


- Using the math and physics he invented, Newton proved that the motion of the planets around the sun is an *ellipse* (Kepler's first law). This is a beautiful example of the traditional, pencil and paper approach to theoretical physics.
- Once you have three or more objects involved, the pencil and paper approach becomes almost impossible.
- To solve the hard problems on a computer, the approach is just like for chess: 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

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



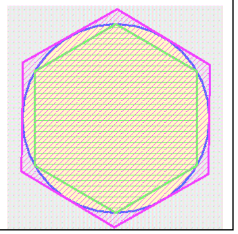
Particle motion: go in a straight line for a short time, then recalculate the direction and speed. The shorter the time intervals, the greater the accuracy.



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:

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



How well does this work?

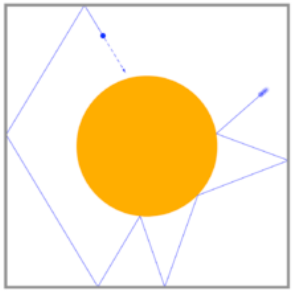
Sometimes, it works extremely well. For example, detailed planetary motion has been simulated for more than 1 billion years!

But: some systems are *chaotic.* For a chaotic system, after simulating for a while your errors blow up!

What is chaos? Studying the motion of a hypothetical system of 3 planets with the same mass in the 1880s, Poincaré discovered that very very tiny errors in how you start the system give huge differences in the results.

A simpler example due to Sinai is "Sinai billiards"

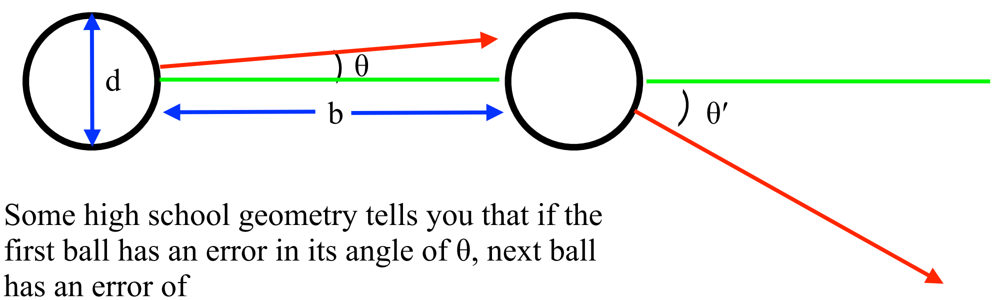
Ordinary billiards also exhibits chaos, which might be useful in "pool hustling"



Sinai Billiards


STA Travel
Wells Fargo Bank
SchoolsFirst FCU

Billiard ball collisions



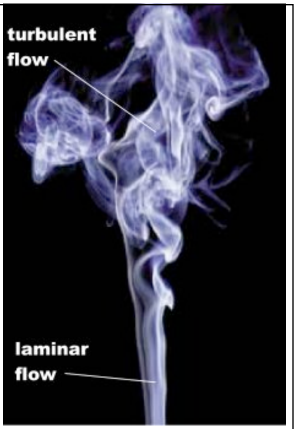
Some high school geometry tells you that if the first ball has an error in its angle of θ, next ball has an error of

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

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

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

Chaos and the weather



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

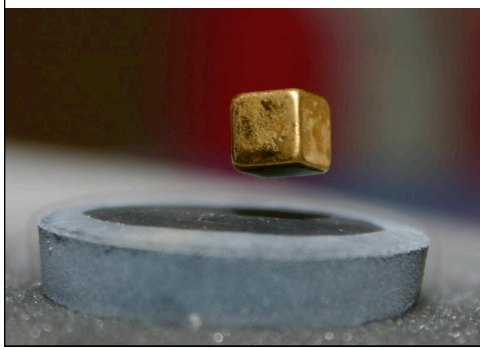
The “butterfly effect” is from a talk given by Lorenz to the AAAS in 1972: “*Predictability: Does the Flap of a Butterfly’s Wings in Brazil set off a Tornado in Texas?”*

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?

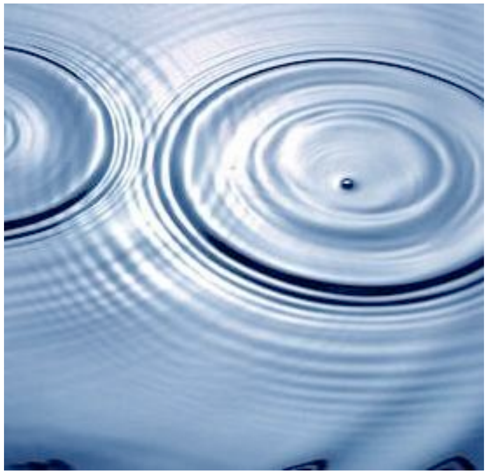
Quantum Mechanics

- 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!

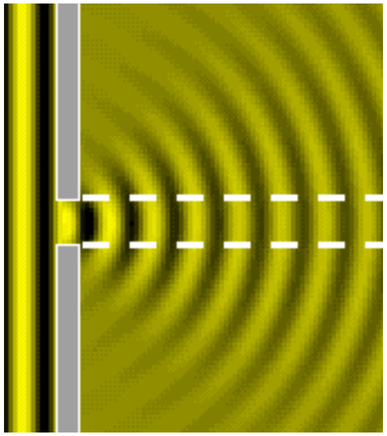


Water waves

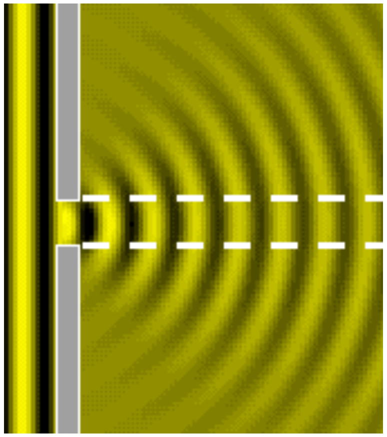
The first step in understanding quantum mechanics is understanding the difference between waves and particles.



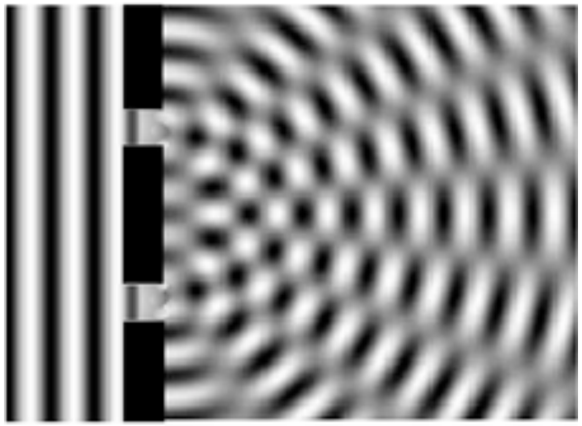
Waves from pebbles in a pond



Straight waves hitting a single small slit make circular waves

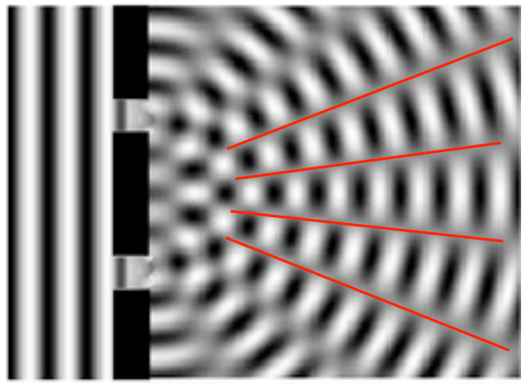


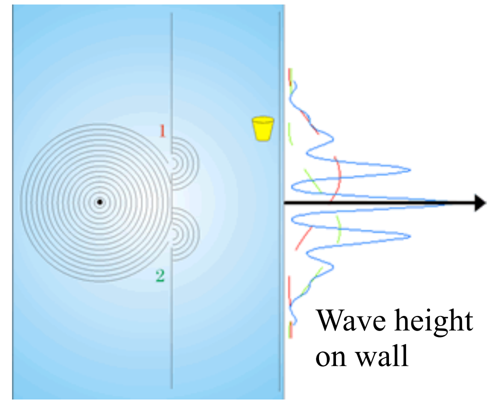
Waves hitting a single slit make circles



Waves hitting two slits: interference

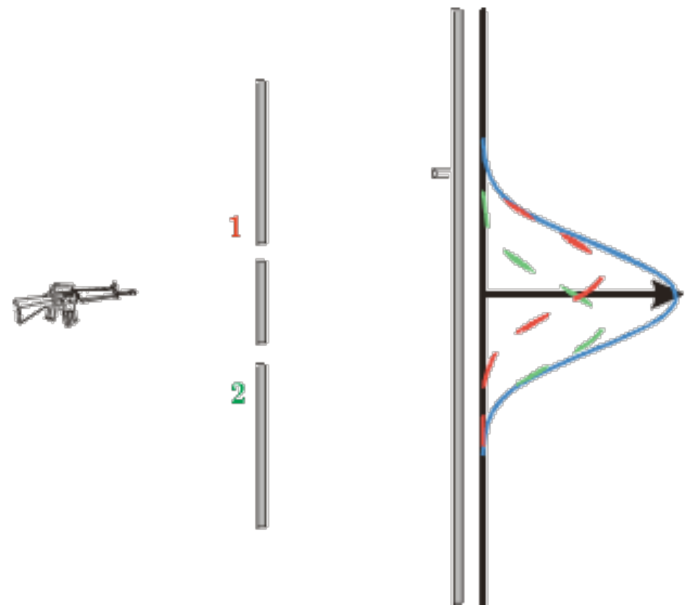
Interference patterns



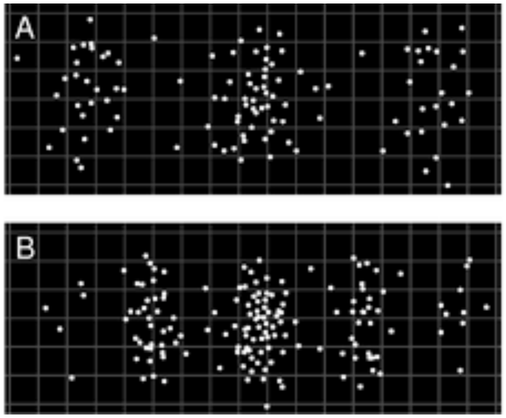


Red lines show where waves cancel

Particles (like bullets) don't have interference patterns



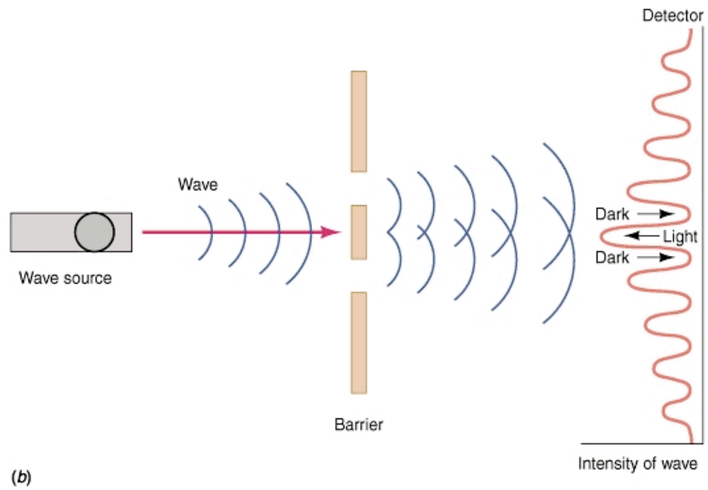
What do electrons do?



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.

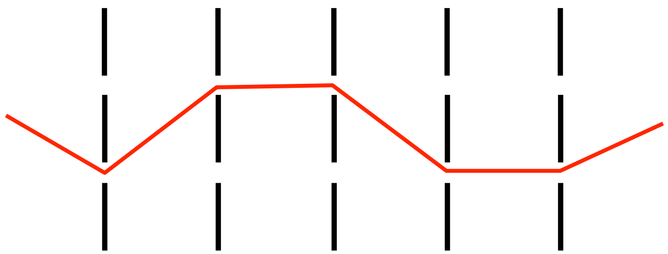


Which slit did the electron go through?

- This sort of question has puzzled physicists for 80 years! Feynman: “no one understands quantum mechanics”
- 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?

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!

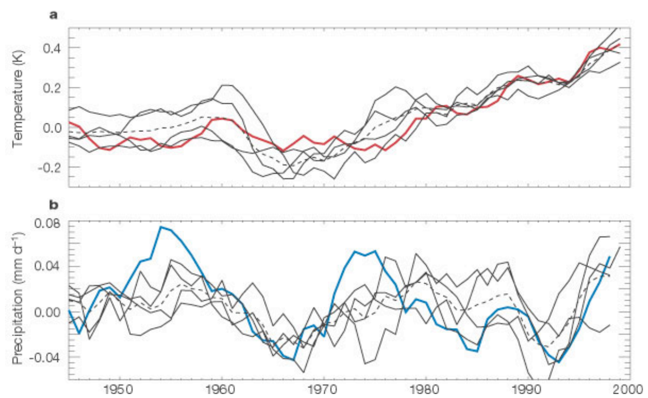
Simulating quantum mechanics is exponentially hard!

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 <u>averages</u> and <u>probabilities</u>. (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



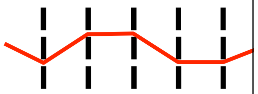
Colored lines: real-world measurments

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...



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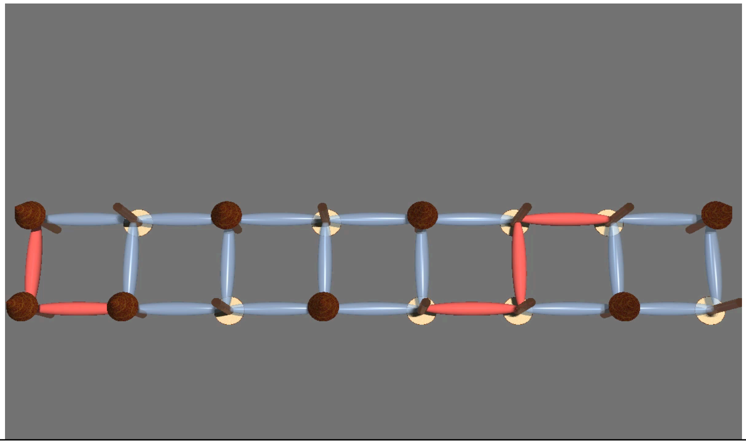
quantum Las Vegas?

Does this quantum Monte Carlo approach 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…
- 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.



Minimally entangled typical thermal states (METTS)

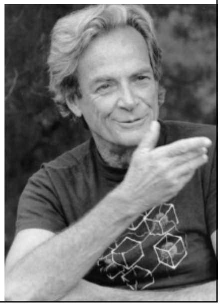
Summary: simulating chaos and quantum mechanics

- 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 much of the difficulty by "rolling the dice", using randomness as an ally in our simulations: ensemble simulations and quantum Monte Carlo.

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



Thanks to:
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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