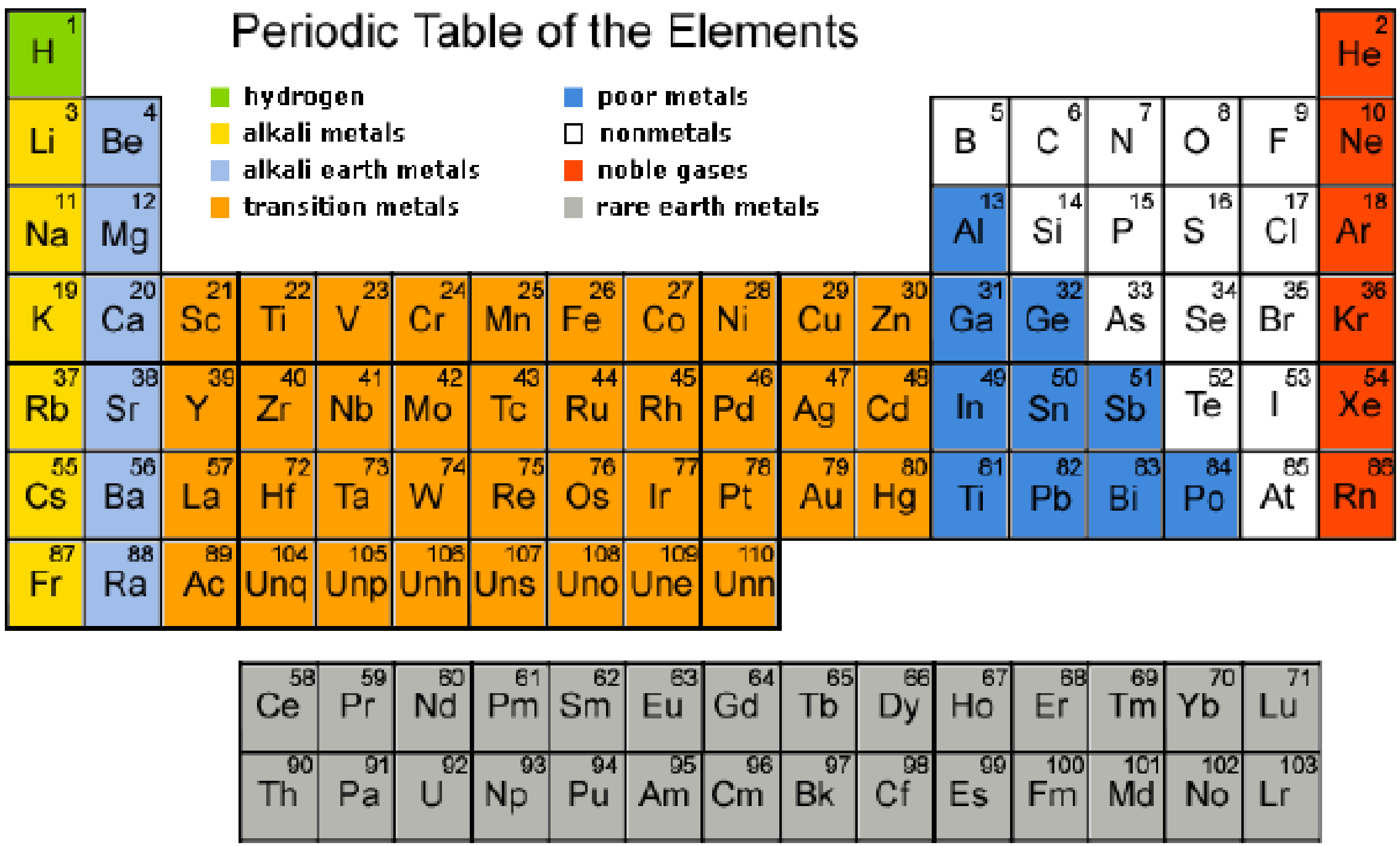
Concepts in Theoretical Physics

Lecture 4: Quantum Mechanics

John D Barrow

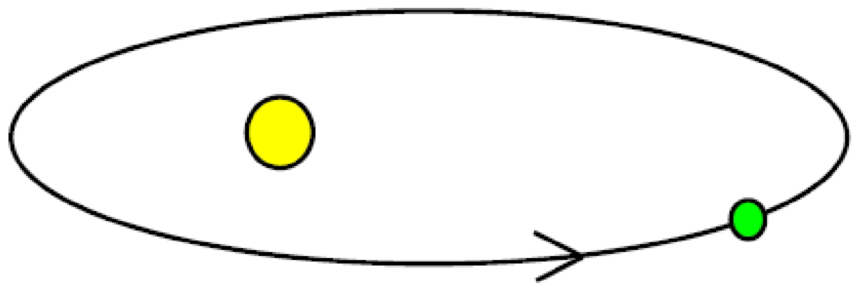
'Everything in the past is a particle.
Everything in the future is a wave'
Freeman Dyson

The whole of atomic physics



Classical electron orbits

- Consider the electron orbiting the proton.
- The classical problem (i.e. F=ma) is exactly the same as a planet orbiting the sun.
- The orbits are ellipses, with the sun (or proton) at one focus.

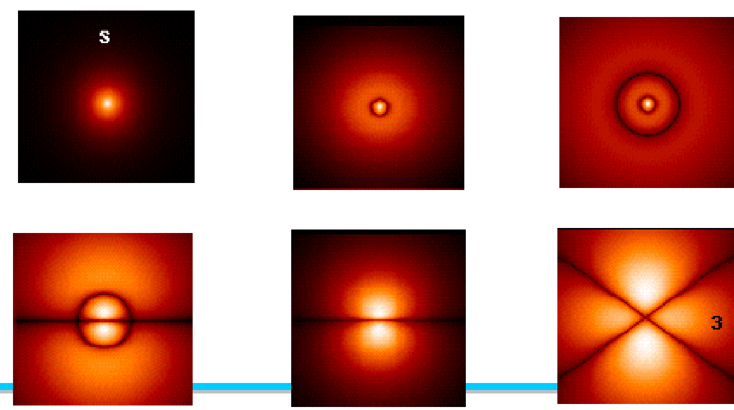


- But there's no restriction on the size or eccentricity of the orbit….that depends only on initial conditions of the problem

$m_e v^2/r = Ze^2/4\pi\varepsilon_0 r^2$, atomic number Z= no. of protons in nucleus, $m_e << m_{pr}$
$v = (Ze^2 /4\pi\varepsilon_0\, mr)^{1/2}$, so we can have <u>any</u> r for some v and all atoms are different!

Quantum electron orbitals

- In quantum mechanics the answer is very different
- The electron can only sit in very particular orbits.
- Yet, in each of these orbits, its position is undetermined. It is smeared out, a wave of probability.

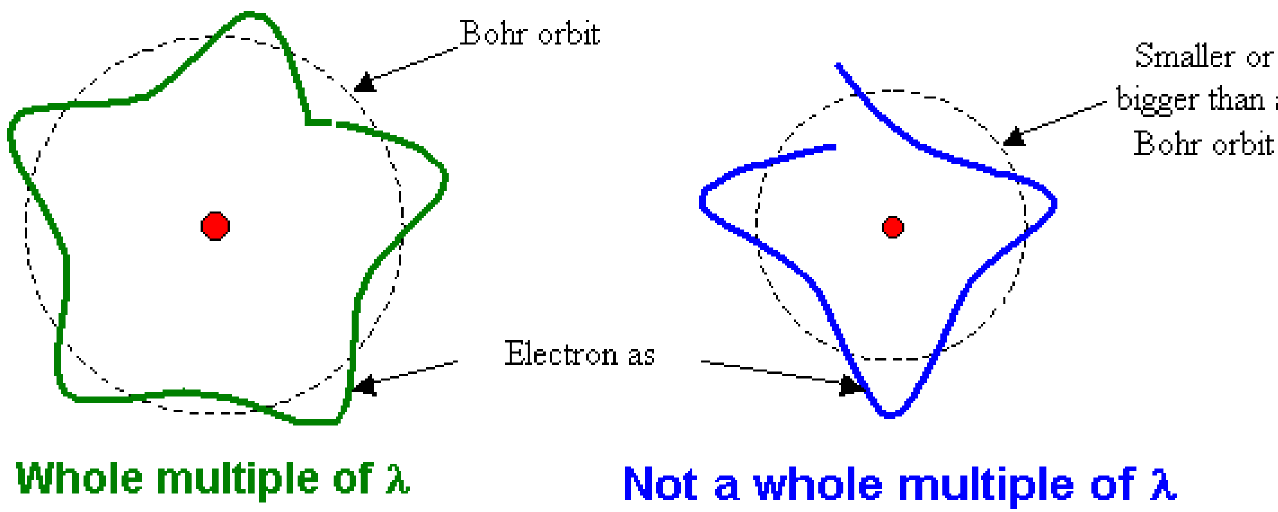


Angular momentum: $mv \times 2\pi r = nh$, n integer, h Planck's constant
$r_n = n^2h^2\varepsilon_0/\pi Ze^2m_e$ quantized orbits and energies $E_n = -Ze^2/8\pi\varepsilon_0 r_n$
This is why there are populations of identical stable atoms

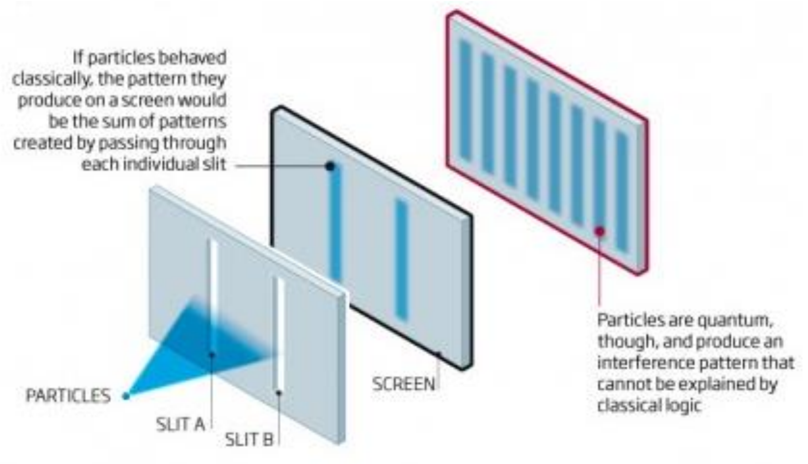
Quantisation condition

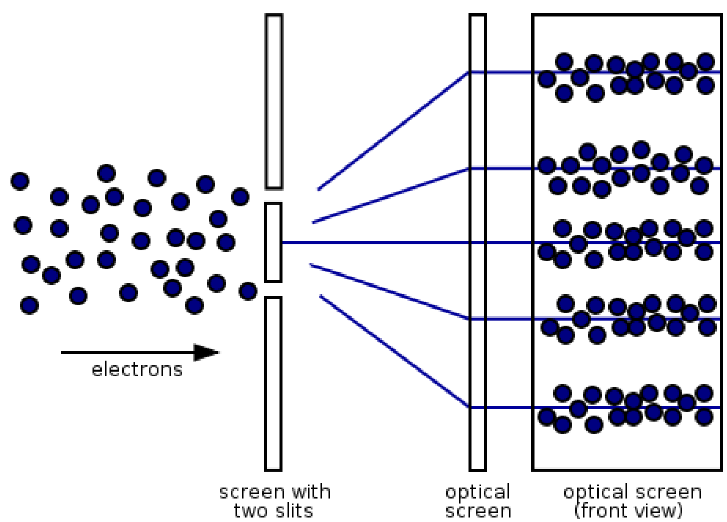
Only whole numbers of quantum wavelengths fit into a circular orbit

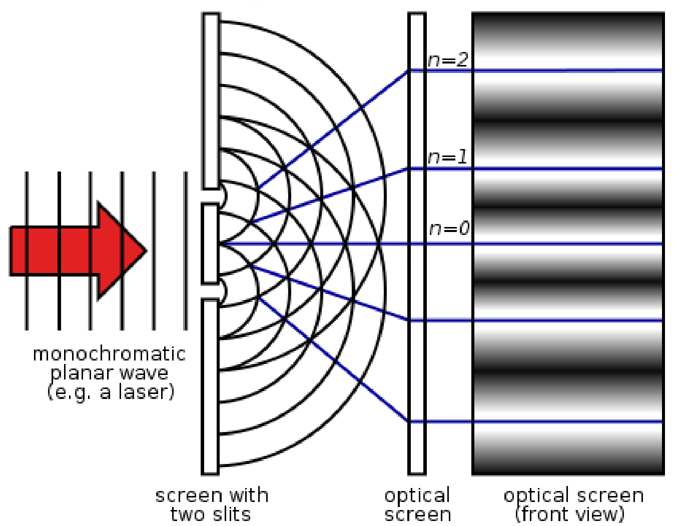
$$\lambda = h/mv$$



The two-slit experiment







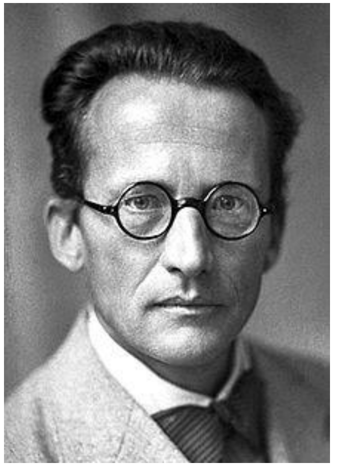
The Mathematical Description

- The mathematical framework of quantum mechanics was covered in “Vectors and Matrices”, with more in next year’s “Linear Algebra”.
- However, this may not be apparent when taking your first “Quantum Mechanics” course next year, where “Differential Equations” will appear more important.

Schrödinger’s Equation

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r},t)\psi(\mathbf{r},t)$$

i is the imaginary number, $\sqrt{-1}$.
$\hbar$ is Planck's constant divided by 2π: 1.05459×10^{-34} joule·second.
$\psi(\mathbf{r},t)$ is the wave function, defined over space and time.
m is the mass of the particle.
∇^2 is the Laplacian operator, $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$.
$V(\mathbf{r},t)$ is the potential energy influencing the particle.



Erwin Schrödinger

Deriving Schrödinger's equation in 1-d

Take a wave of frequency ω moving in the +x direction, k = 2π/λ

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

For a free particle momentum p = ħk, energy E = ħω this means

$$\frac{\partial^2\Psi}{\partial x^2} = -k^2\Psi$$

which can be written, using $E = p^2/2m = \hbar^2 k^2/2m$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = \frac{p^2}{2m}\Psi.$$

Similarly

$$\frac{\partial\Psi}{\partial t} = -i\omega\Psi$$

which can be written, using $E = \hbar\omega$:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hbar\omega\psi = E\Psi$$

We now generalize this to the situation in which there is both a kinetic energy ar potential energy present, then $E = p^2/2m + V(x)$ so that

$$E\Psi = \frac{p^2}{2m}\Psi + V(x)\Psi \qquad ($$

where Ψ is now the wave function of a particle moving in the presence of a potential V

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\Psi = i\hbar\frac{\partial\psi}{\partial t}$$

States

- The *state* of a system consists of all the information that's required to determine the state of the system at all times in the future

- In Classical Mechanics, the state of a system is by given the positions and momenta of all the particles.

The Superposition Principle

- In quantum mechanics, the state lives in a vector space. This means that we are allowed to add and subtract states…something which makes no sense in classical mechanics.

$\psi =$  + 

- The vector ψ is called the *wavefunction*. It is typically a vector in an infinite dimensional vector space, known as a *Hilbert space*.

Eigenvectors and eigenvalues

- While the state of the system is a vector, the measurements that we do on a system are matrices. We have a different matrix for each type of measurement: e.g. position, momentum, energy…

- The possible outcomes of a measurement are the eigenvalues of the matrix.

$$\underbrace{H}_{\text{matrix}}\psi = \underbrace{E}_{\text{eigenvalue}}\psi$$

- For example: if H is the matrix representing a measurement of energy, then the eigenvalues E are the possible outcomes of that measurement

- When H is energy, this is known as the *Schrodinger Equation.*

Probabilities

Max Born

- What happens if our state ψ is not an eigenvector of the matrix we are measuring?
- Then the measurement could give any one of the eigenvalues E_i . Each occurs with some probability
- We expand our state in a basis of eigenvectors of H.

$$\underbrace{\psi}_{\text{actual state}} = \sum_i c_i \underbrace{\psi_i}_{\text{eigenvectors}}$$

- Then the probability of the measurement giving E_i is

$$Prob(E_i) = \frac{|c_i|^2}{\sum_j |c_j|^2}$$

The Inevitability of Uncertainty

- Most matrices have different eigenvectors. This means that if the state is in an eigenvector of one matrix, it is unlikely to be in an eigenvector of a different matrix.

- So if one type of measurement is certain, another type becomes uncertain.

- This is *Heisenberg's Uncertainty Principle.* If we know, say, the position of the particle then it's momentum becomes uncertain. And vice versa.

Heisenberg's Uncertainty Principle

- If Δx is position uncertainty and Δp is uncertainty in momentum then

$$\Delta x \Delta p > 1/2\ \hbar$$

- Another dimensional equivalent (not rigorous – time is not an operator) governs energy and time uncertainties

$$\Delta E\ \Delta t > 1/2\ \hbar$$

- This 'uncertainty' is deeper than limits on practical measurements.

Wigner's Clock Inequality

- There is a smallest 'clock'
- Clock of mass M has quantum position uncertainty Δx and momentum uncertainty at least $\hbar/\Delta x$
- Suppose clock can resolve a smallest time interval τ and must run for total time T. After time t, the uncertainty in position of the clock is $\Delta x' = \Delta x + \hbar t/(M\Delta x)$. This is a minimum when $\Delta x = (\hbar t/M)^{1/2}$. To run the clock accurately for time T, it must be bigger than $(\hbar T/M)^{1/2}$. To keep time ('tick') with an accuracy τ we need $\Delta x' < c\tau$, so there is a minimum clock mass

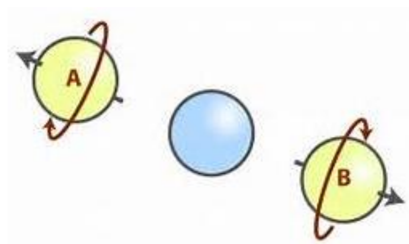
$$M > (4\,\hbar/c^2\tau)(T/\tau)$$

- A stronger bound than the E-t uncertainty principle by T/τ
- Relevant for bacteria, nano machines and black holes

Entanglement – “quantum weirdness”

- To end, let’s look at one of the more bewildering aspects of quantum mechanics. It is the fact that strange correlations can exist between experiments. This subject is usually called *entanglement*.

• Einstein, Podolsky and Rosen (‘EPR’) tried to use it to disprove quantum mechanics in 1935 because they thought it’s predictions were too outrageous to be true:



• In 1964 John Bell proposed a specific experiments to test whether entanglement occurs.
• In 1982 Alain Aspect et al did that experiment.

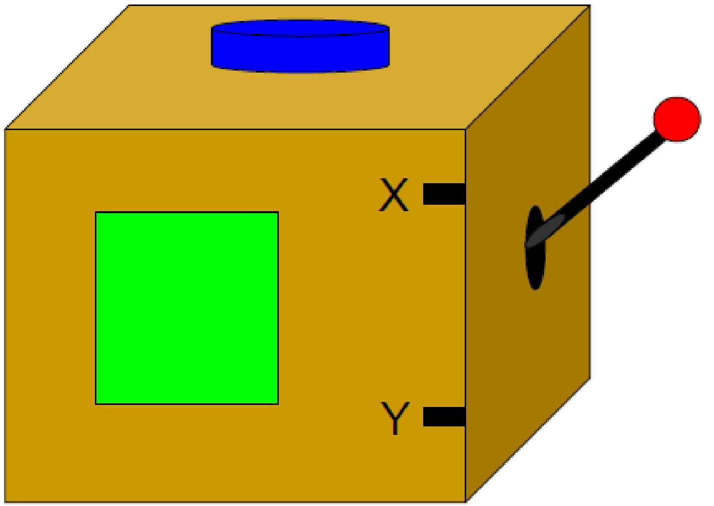
Quantum reality turns out to be much stranger than your (non-quantum) imaginings

The Greenberger, Home and Zeilinger (GHZ) Experiment

- Three scientists are each sitting in a lab, separated in spacetime.

- Every minute, they receive a package sent from a mysterious central station. They are told what they have to do…

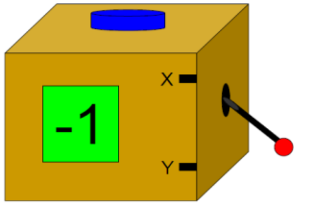
Each scientist has a machine like this that has two settings, X and Y, and can give outcome +1 or -1 from a measurement



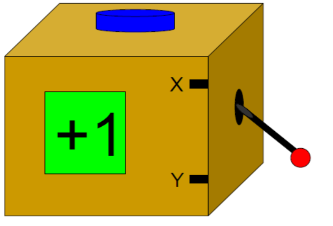
- Chose the setting for switch
- Place the sample in the machine
- Press the button, and record whether the result is +1 or -1

Make many measurements

- The scientists are not told what's in the packages
  - They could be blood samples, with the machine testing for high/low glucose when the switch is on X, and high/low cholesterol when the switch is on Y.
  - They could be elementary particles
  - Or the whole thing could just be a hoax with the machine flashing up +1/-1 at random



- Each measurement is recorded until each scientist has a list that looks like this but with a bazillion entries



X	X	Y	X	Y	Y	X	Y	Y	Y	Y	X	X	Y	X
+1	-1	+1	+1	-1	-1	-1	+1	+1	-1	+1	-1	+1	+1	+1

Looking for a pattern

- Now the scientists get together and start looking for correlations in the measurements. They notice the following.
- Whenever one person measured X, and other two measured Y, the results *always* multiply to +1

$$X_1 Y_2 Y_3 = Y_1 X_2 Y_3 = Y_1 Y_2 X_3 = +1$$

This means the first person measured X, while the second and third people measured Y

Maybe this was because all 3 got result +1, or one got +1 and other two got -1 etc

The eight possibilities

- Maybe this occurred because all three got the result +1; or perhaps one got +1 and the other two got -1. There are 8 ways that this could have happened

$$\begin{pmatrix} X_1 = + & Y_1 = + \\ X_2 = + & Y_2 = + \\ X_3 = + & Y_3 = + \end{pmatrix} \quad \begin{pmatrix} X_1 = - & Y_1 = - \\ X_2 = - & Y_2 = - \\ X_3 = + & Y_3 = + \end{pmatrix} \quad \begin{pmatrix} X_1 = - & Y_1 = + \\ X_2 = - & Y_2 = + \\ X_3 = + & Y_3 = - \end{pmatrix}$$

$$\begin{pmatrix} X_1 = - & Y_1 = - \\ X_2 = + & Y_2 = + \\ X_3 = - & Y_3 = - \end{pmatrix} \quad \begin{pmatrix} X_1 = - & Y_1 = + \\ X_2 = + & Y_2 = - \\ X_3 = - & Y_3 = + \end{pmatrix} \quad \begin{pmatrix} X_1 = + & Y_1 = - \\ X_2 = + & Y_2 = - \\ X_3 = + & Y_3 = - \end{pmatrix}$$

$$\begin{pmatrix} X_1 = + & Y_1 = + \\ X_2 = - & Y_2 = - \\ X_3 = - & Y_3 = - \end{pmatrix} \quad \begin{pmatrix} X_1 = + & Y_1 = - \\ X_2 = - & Y_2 = + \\ X_3 = - & Y_3 = + \end{pmatrix}$$

A Prediction

- But this gives a prediction….whenever all three scientists measured X, the results multiplied together *must* give +1

$$
\begin{aligned}
(X_1Y_2Y_3)(Y_1X_2Y_3)(Y_1Y_2X_3) &= X_1X_2X_3(Y_1Y_2Y_3)^2 \\
&= X_1X_2X_3 \\
&= +1
\end{aligned}
$$

- This is so simple, it couldn't even be called a law of physics. It follows from our most basic ideas about how the universe works.

[Just note that $X_1 = Y_2Y_3$ and $X_2 = Y_1Y_3$ and $X_3 = Y_1Y_2$ by multiplying across the above relation $X_1Y_2Y_3 = Y_1X_2Y_3 = Y_1Y_2X_3 = +1$]

The shocking truth

- This experiment has been done.*
- The things measured were the polarization of photons. (Spins of elementary particles would work just as well).
- The results are

$$X_1 Y_2 Y_3 = Y_1 X_2 Y_3 = Y_1 Y_2 X_3 = +1$$

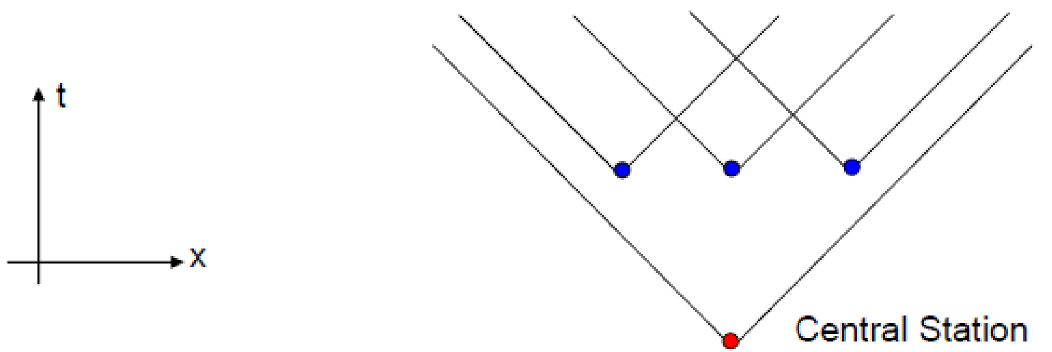
$$X_1 X_2 X_3 = -1$$

- The very basic (classical) intuition for how the universe works is *wrong!*

* Pan et. al. Nature 2000, Feb 3;403(6769): 515-519

Spooky faster-than-light effects ?

- An implicit assumption is that the measurements are performed independently, so that experiment 2 has no way of knowing whether the switch on experiment 1 is set to X or Y.
- But we can guarantee that this is true, by placing the scientists at space-like separated points.



- It appears that these correlations require information to be transmitted faster than light!

Quantum reality replaces common sense

- The resolution to the paradox is that we assumed the packages leaving the central station had definite assignments, e.g.

$$\begin{pmatrix} X_1 = - & Y_1 = + \\ X_2 = + & Y_2 = - \\ X_3 = - & Y_3 = + \end{pmatrix}$$

- But in the quantum world, we cannot give definite assignments to all possible measurements. The package that arrived didn't have both X and Y assigned at the same time.

- The GHZ correlations are *almost* nonlocal. In a classical world, the only way you could get such correlations is by non-locality, which implies transmission of information faster than the speed of light.

- But our world is quantum. And such correlations are allowed without faster-than-light communication.

What were they measuring?

- They were measuring spins of particles. The measurement matrices are

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- You can check that these have eigenvalues +1 and -1, corresponding to the measurements
  - But X and Y do not have the same eigenvectors

- The state that the central station was sending is neither an eigenvector of X nor Y. It is

$$\Psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The resolution

- The state that the central station was sending is neither an eigenvector of X nor Y. It is

$$\Psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- This is an eigenvector of XYY and YXY and YYX.
- And, importantly, it is an eigenvector of XXX.
- Exercise: Check that this gives rise to the observed correlations.

The spin states of the three particles were not really independent.
They were 'entangled' in the state Ψ.
No matter how far separated our scientists are,
this entanglement of the spin states shows up in their measurements.

This non-locality is how the quantum world is

Further reading

- L. Susskind and A. Friedman *Quantum Mechanics: the theoretical minimum*, Basic Books, (2015)
- P.C.W. Davies and D.S. Betts, *Quantum Mechanics,* 2nd edn Springer, (1994)
- A. Zeilinger, *Dance of the Photons*, Farrar, Straus and Giroux, (2010)
- N.D. Mermin, Quantum mysteries revisited, American Journal of Physics 58, 731-734 (Aug 1990). Online at http://aapt.scitation.org/doi/10.1119/1.16503
- Greenberger, Home and Zeilinger, https://www.physicsforums.com/insights/greenberger-horne-zeilinger-experiment/
- Pan et al Nature 403, 515-9 (2000) and Pan, J., Bouwmeester, D., Daniell, M., Weinfurter, H., & Zeilinger, Z.: Experimental test of quantum nonlocality in three-photon Greenberger-Horne-Zeilinger entanglement. Nature 403, 515-519 (3 Feb 2000).