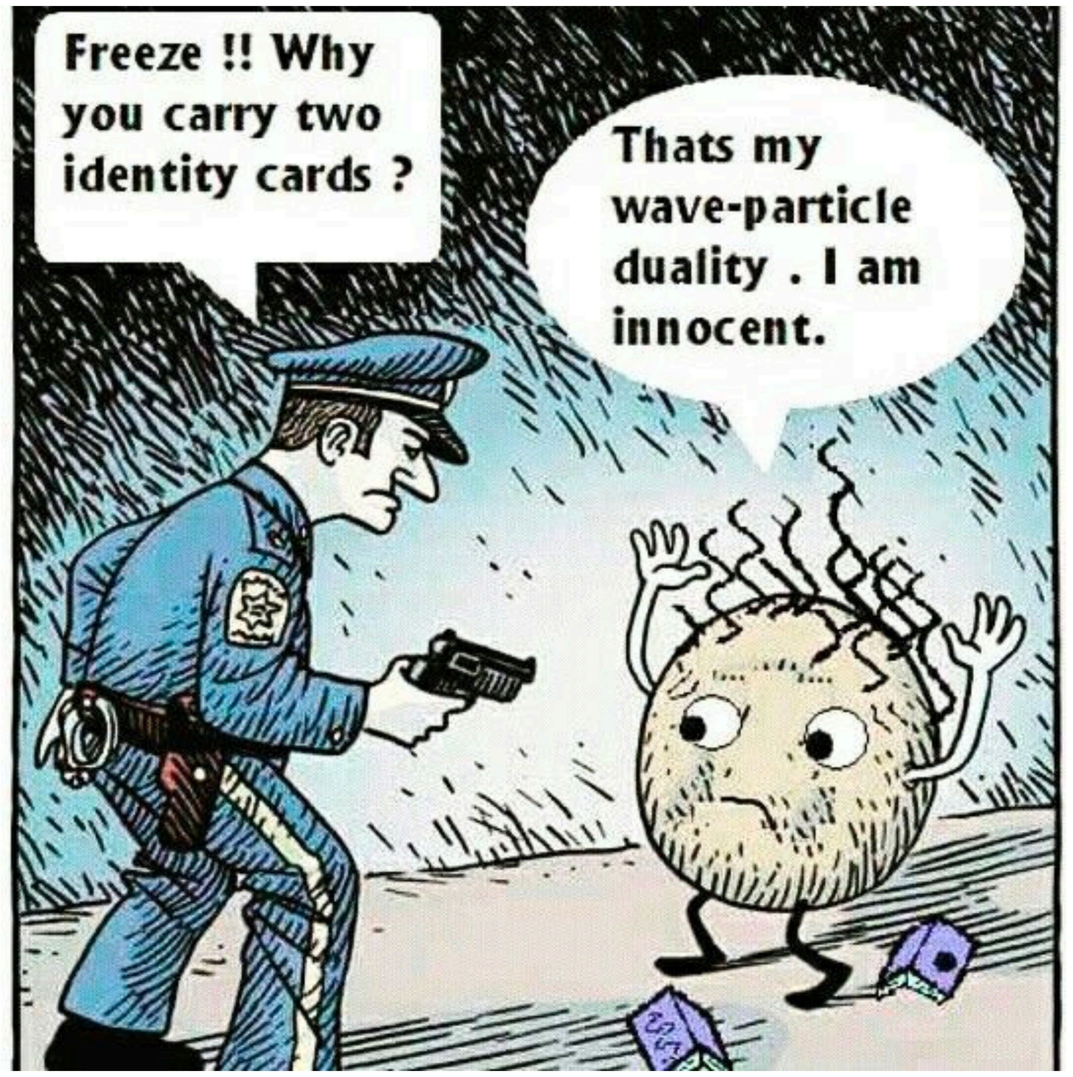
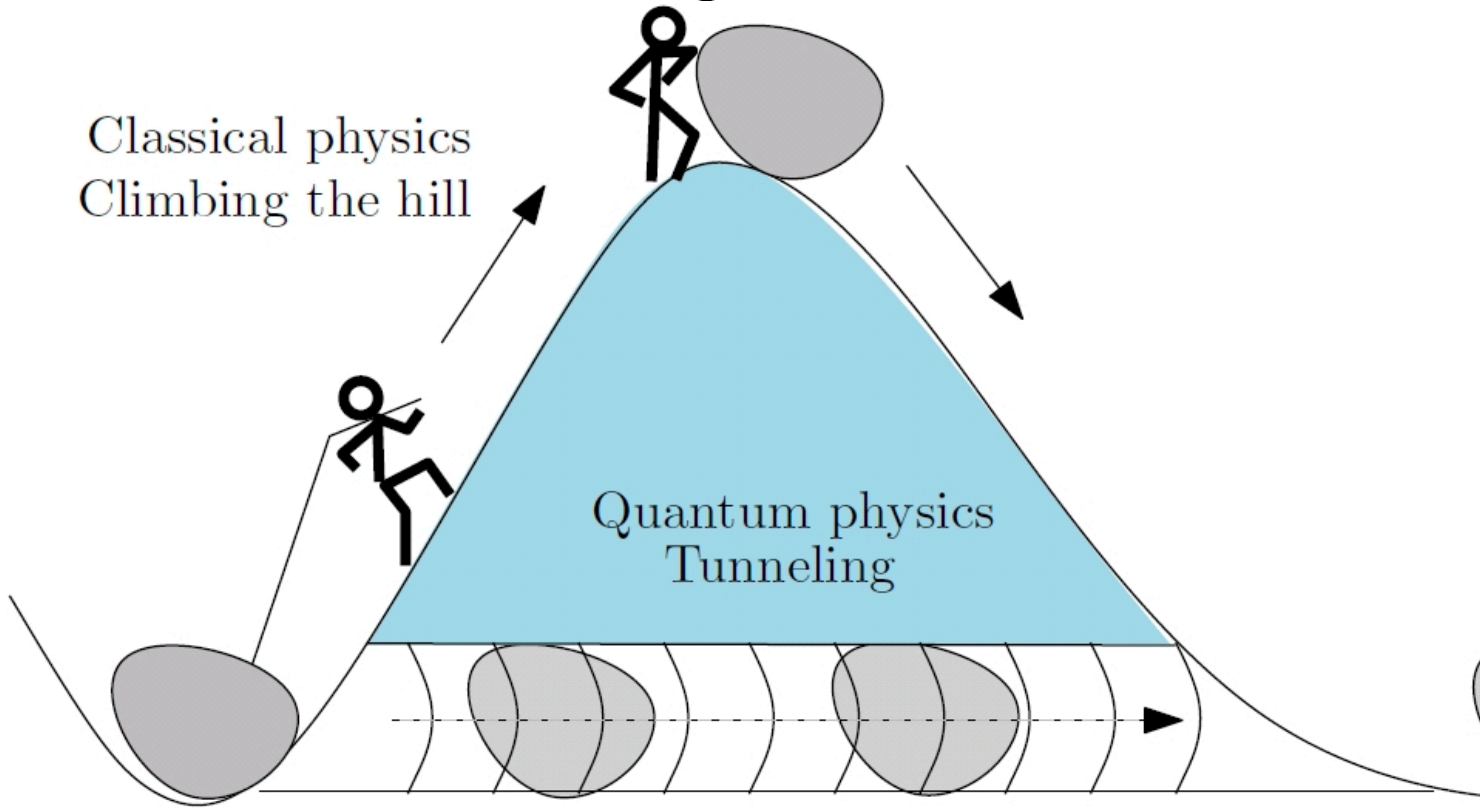
Quantum Mechanics Introduction

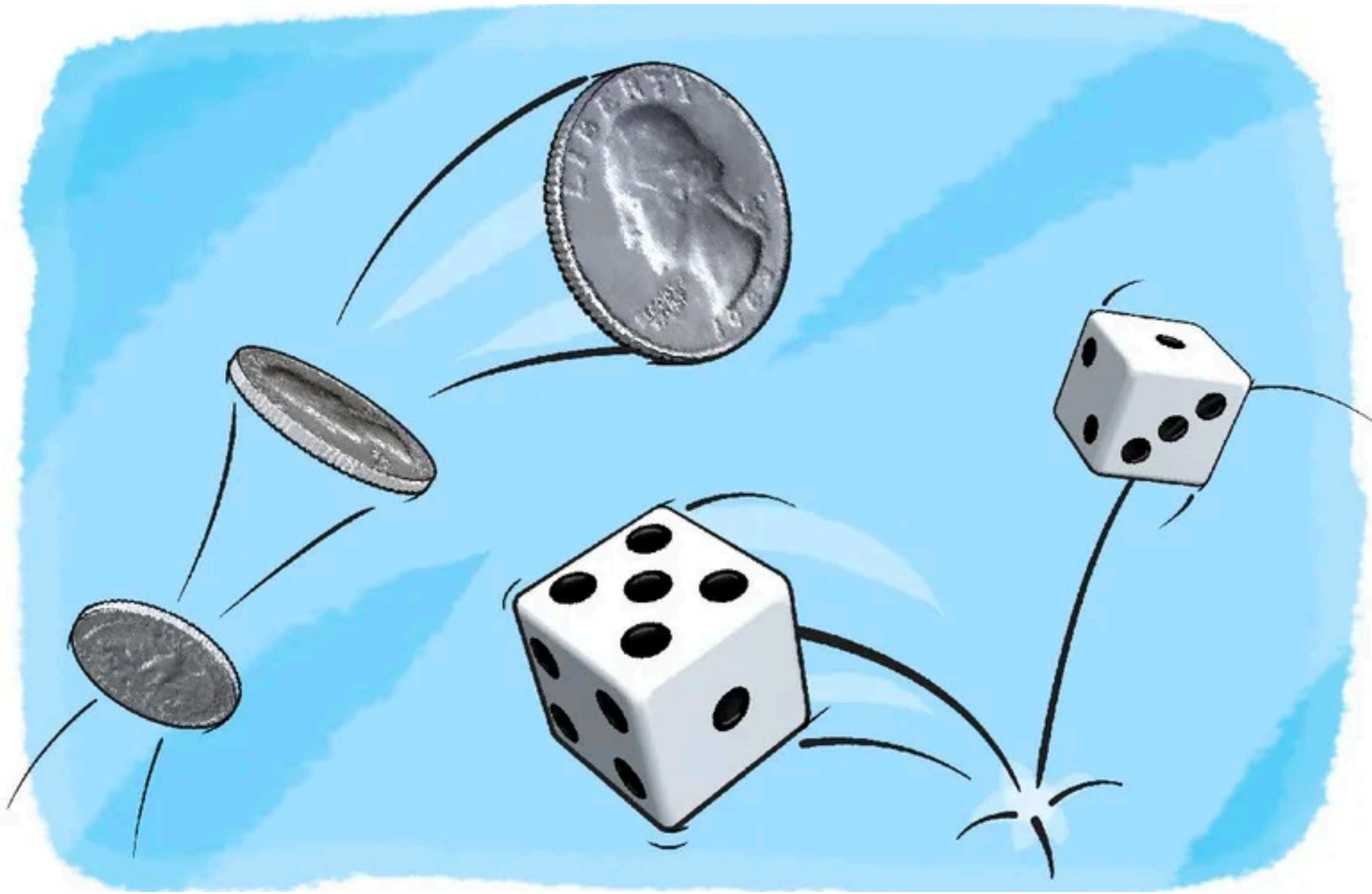
Quantum Mechanic



- Departure from classical mechanics
- Undoubtedly the correct description of the Universe we inhabit
- QM answers old and very basic questions: why is matter stable? Why does the sunshine and why is it yellow?
- But also opens up vistas that we didn't previously know existed: novel states of matter, entanglement: revised understanding of the meaning of information and what one can achieve with it



Probabilistic Nature



- QM gives the right answers but at a cost.
- The answers are always **statistical** in nature.
- There are few certainties in Quantum World.
- In classical world we can always eliminate the uncertainties. In classical Physics **“Knowledge is Power”**
- Classical probabilities are always about our **Ignorance,** classical system that appears random does so because it is somehow difficult, but never impossible, for us to know what’s going on

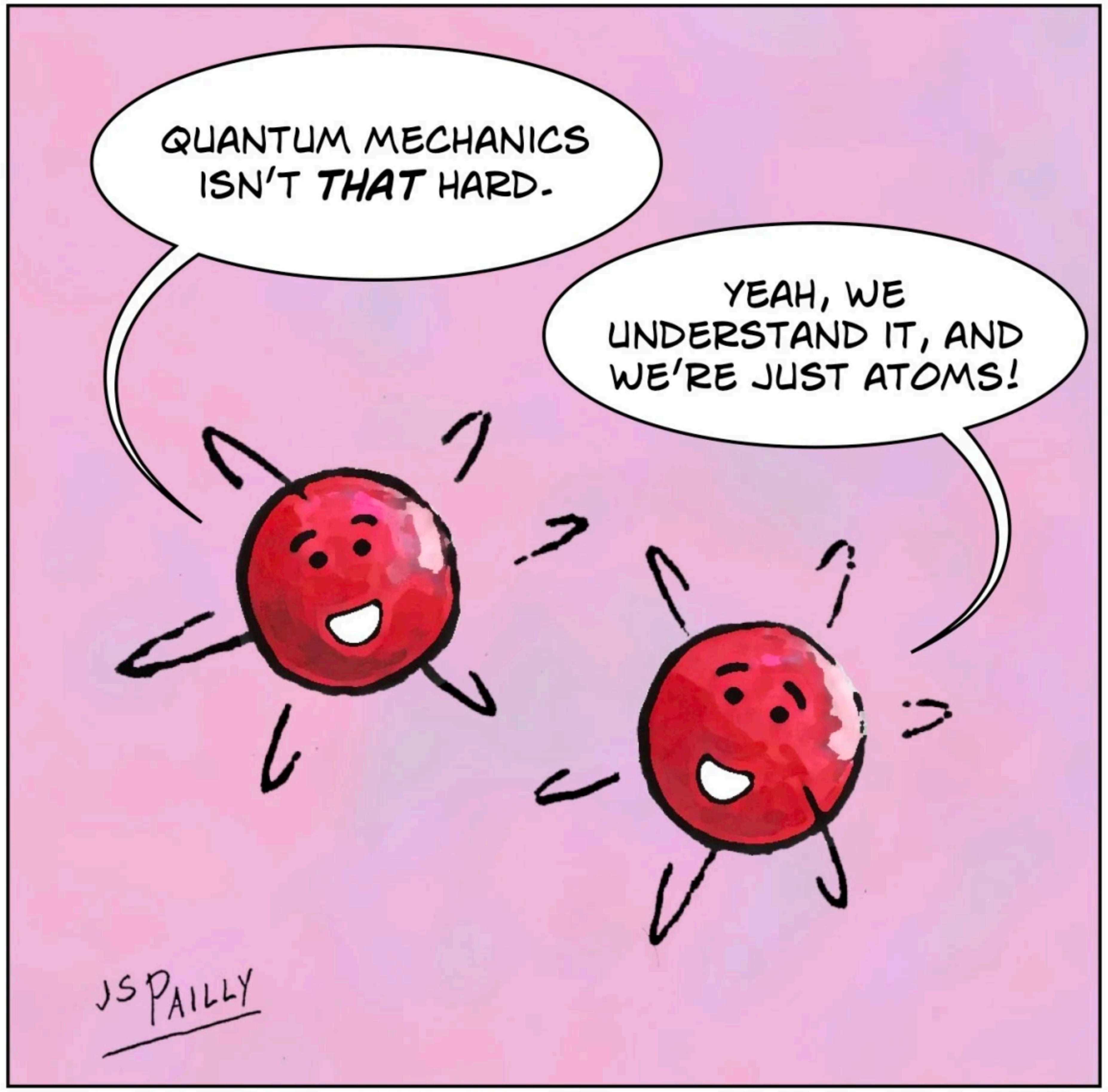
Randomness

- Randomness is real in QM

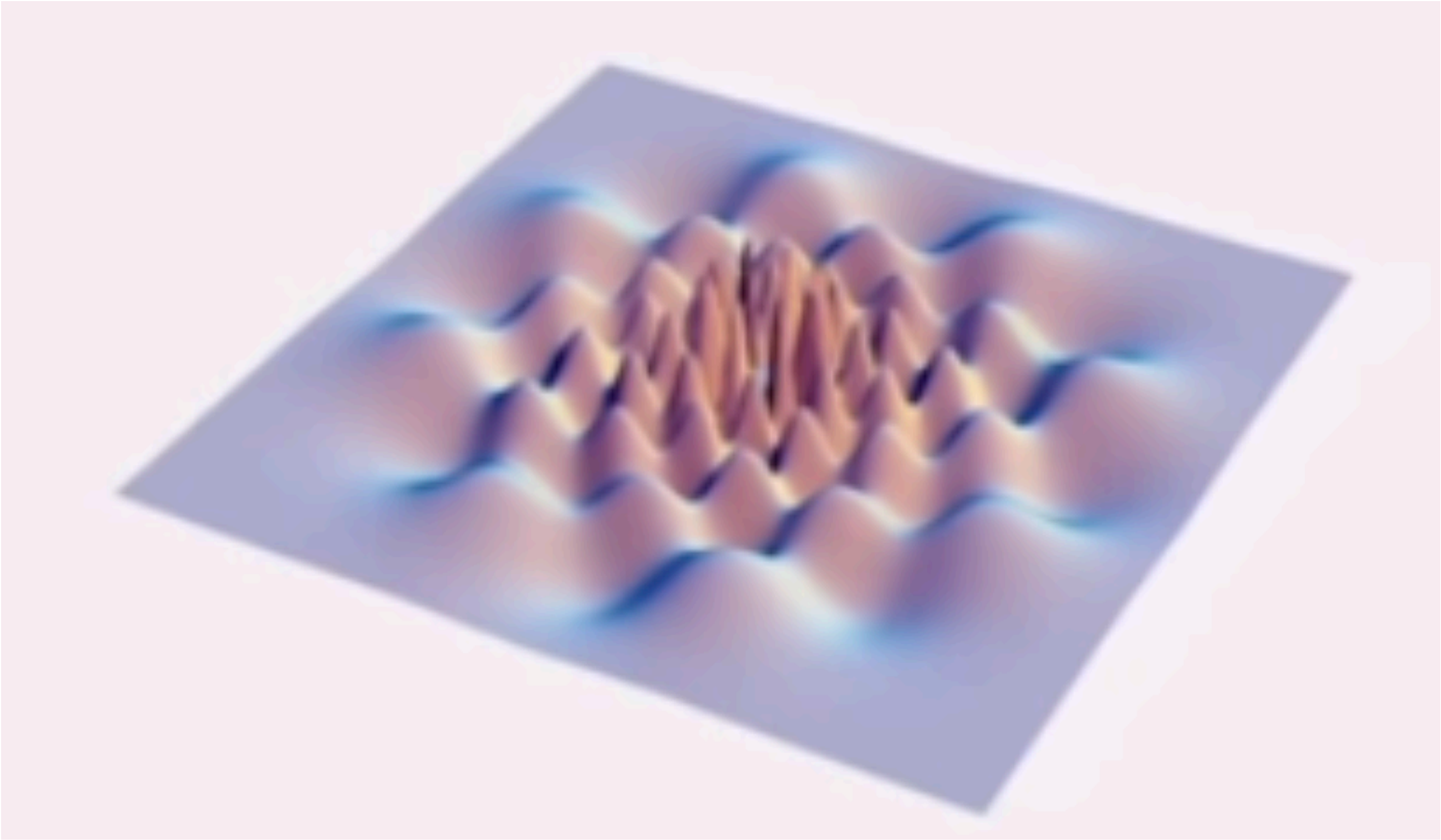
- No way to gain some illicit knowledge of underlying quantum properties that would reduce the uncertainty.

- For example, if the particle has probability 1/2 to be in one place and 1/2 to be elsewhere, this may well be because the particle *really is in both places at the same time.*

- Any attempt to eliminate the quantum certainty will simply shift it like a bubble in wallpaper, elsewhere.



The Wavefunction



- Need to introduce entire new framework in QM
- How we describe the *state* of the system.
- The state is the information that tells us all we need to know about the system at a fixed time, with the idea that the laws of physics will then dictate how the state evolves at all later times.
- We consider particle moving in $\mathbf{R}^3$

State in Classical World

- In classical world, the state of the particle is determined by its position $\mathbf{x}$ and velocity $\mathbf{v} = \dot{\mathbf{x}}$.
- Specify both information at some time t_0 and you can use the equation of motion, $\mathbf{F} = m\ddot{\mathbf{x}}$ to determine $\mathbf{x}(t)$ and $\mathbf{v}(t)$.
- Equation of motion is the second order differential equation so we need to specify two integration constants to get a unique solution

State in Quantum World

- In the quantum world, the state of a particle is determined by its wavefunction. This is a complex valued function

$$\psi(\mathbf{x}, t)$$

- If you know the wave function at some time t_0 then you have all the information that you need to determine the state at all other times.

- The velocity information of the particle should also be contained in the wavefunction

Interpretation of the wavefuntion

- The mode-square of the wave function tells us the probability that we will find a particle at a given time. The probability density for a particle to sit at point $\mathbf{x}$ is : $P(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2$

- This is known as *Born rule.*

- From the probability density you can compute the actual probability by multiplying it by a volume: the probability that the particle sits in some small volume dV centred around $\mathbf{x}$ is $P(\mathbf{x}, t)$dV

Does probability arise because of our ignorance?

- In all other realms of science, probability arises because of our ignorance.
- If you throw a dice and know its initial state with complete precision, then there is no doubt about what will happen.
- Once the dice leaves your hand, the probability that you will roll a six is either 0 or 1.
- If you were really good at solving differential equations, you could figure out the answer. But in reality we don't have a knowledge of the initial conditions, so we just accept our ignorance and admit that the probability of rolling a six is 1/6.

Does probability arise because of our ignorance?

- THIS IS NOT THE CASE IN QUANTUM MECHANICS!

- The state $\psi(\mathbf{x}, t)$ contains all the information and the probabilistic interpretation is not because of our ignorance but instead due to an inherent randomness in the quantum world.

- The wave function doesn't describe a *field,* it is just wave of probability.

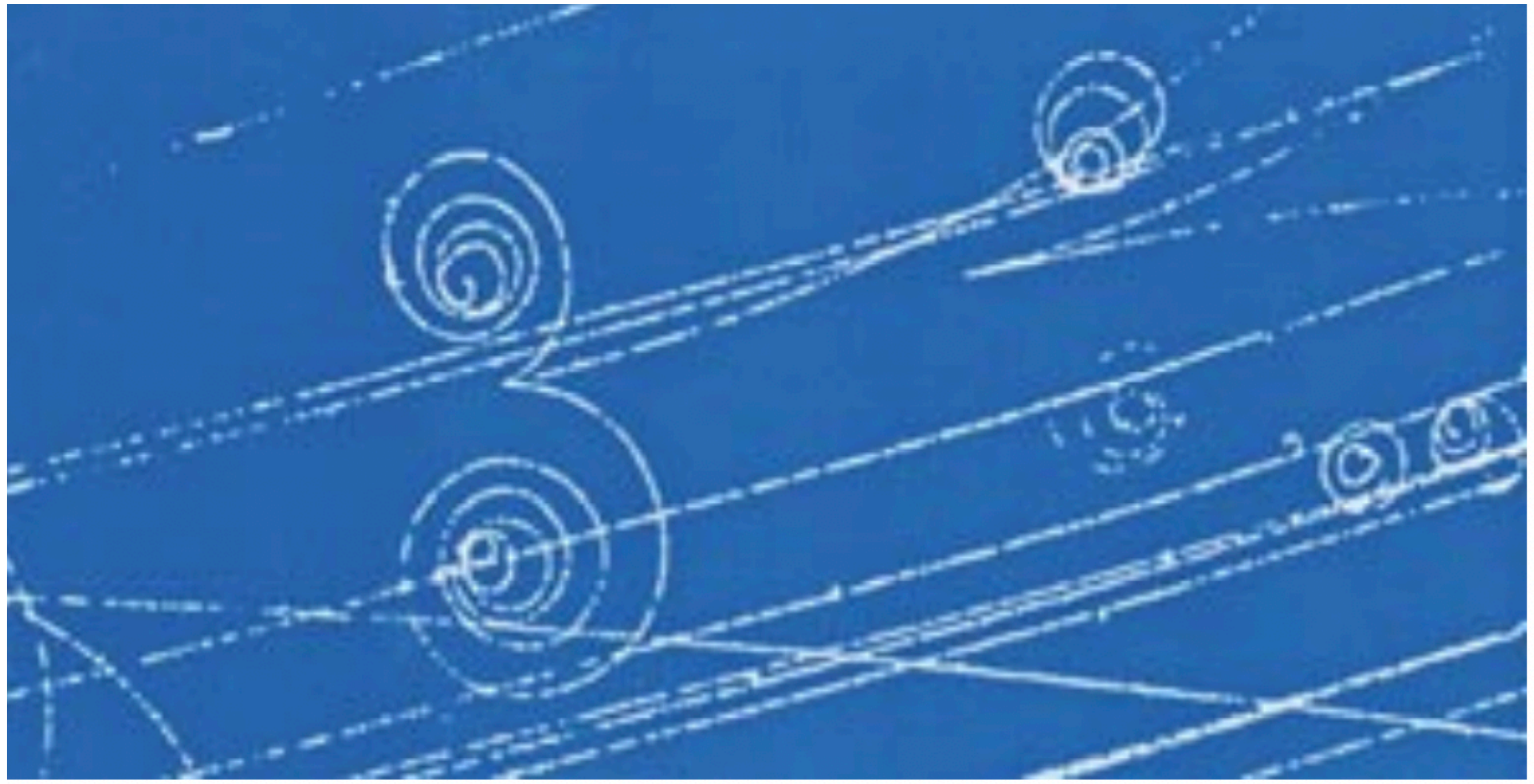
- Any device you use to measure the presence of the particle will tell you if it is present or not. It will not tell you that it is present a little bit here and little bit there.

- In any experiment you only detect particles with only definite trajectories

- The fast travelling particles move in approximately straight lines, while those that are slower spiral in circles due to an applied magnetic field.

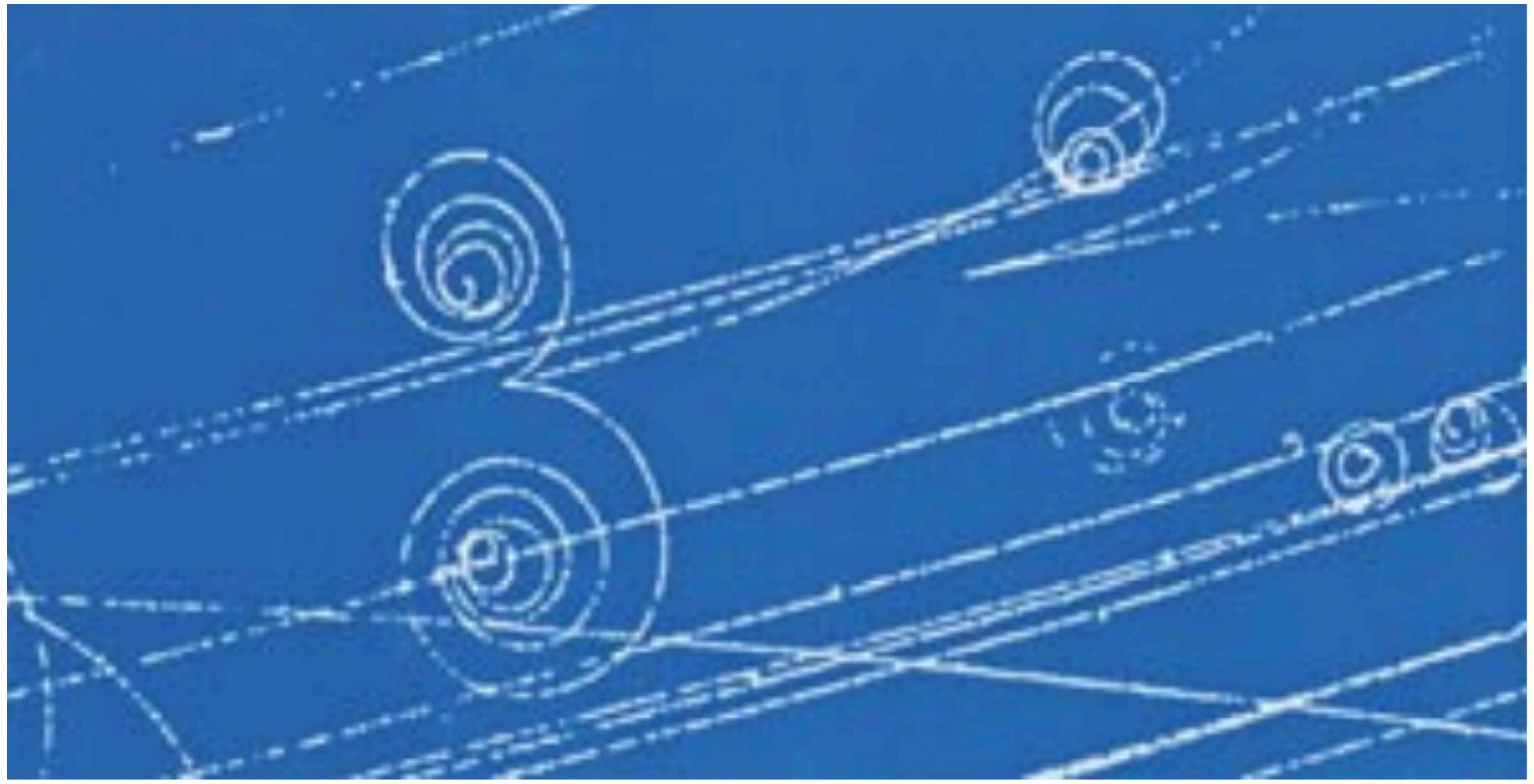
- For our purposes, the key point is that when the particles entered the detector, they were described by a wavefunction that was spread out over a large part of space.

- Yet, the particles don't appear as fluffy, insubstantial clouds of probability. Instead, they leave clear tracks, with a definite trajectory.



- The introduction of probability at such a fundamental level means that we must abandon the idea of predicting, with certainty, what will happen in a given experiment. There is no way to say when and where the spirals will appear in the picture above.

- We can only compute the **likelihood** for this to happen.



Reality is, at heart, probabilistic.

Wavefunction Normalisation

- The probabilistic nature means that the wave function should fulfil the following description: $\int P(\mathbf{x}, t) \mathrm{d}^3\mathbf{x} = \int |\psi(\mathbf{x}, t)|^2 \mathrm{d}^3\mathbf{x} = 1$

- Suppose we have $\psi(\mathbf{x}, t)$ that isn't normalised : $\int |\psi(\mathbf{x}, t)|^2 \mathrm{d}^3\mathbf{x} = N < \infty$

- In this case, we can always normalised the wave function like this:
$$\Psi(\mathbf{x}, t) = \frac{1}{\sqrt{N}}\psi(\mathbf{x}, t)$$

- Functions that cannot be normalised have no use, as they do not have any probabilistic interpretation.

Complex Phase

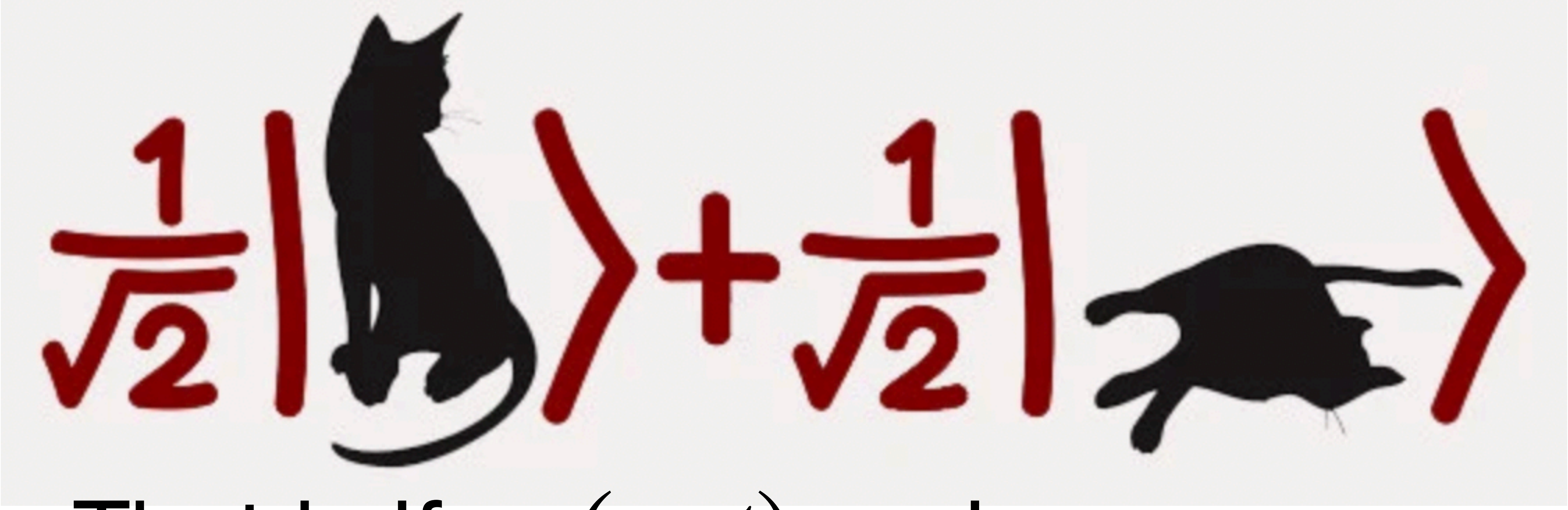
- Two wavefunctions that differ by a constant, complex phase should actually be viewed as describing equivalent states: $\psi(\mathbf{x}, t) \equiv e^{i\alpha}\psi(\mathbf{x}, t)$

- Note that this doesn't change the probability distribution. Note that this α is a real constant. However, if it is a function of spatial coordinates, $\alpha(\mathbf{x})$, then it will change some other observables despite not changing the probability distribution.

- It is sometimes useful think of states as the collection of normalisable, complex functions with the equivalence relation: $\psi(\mathbf{x}, t) = \lambda\psi(\mathbf{x}, t)$

ψ and $\lambda\psi$ describe the same physical state

Superposition



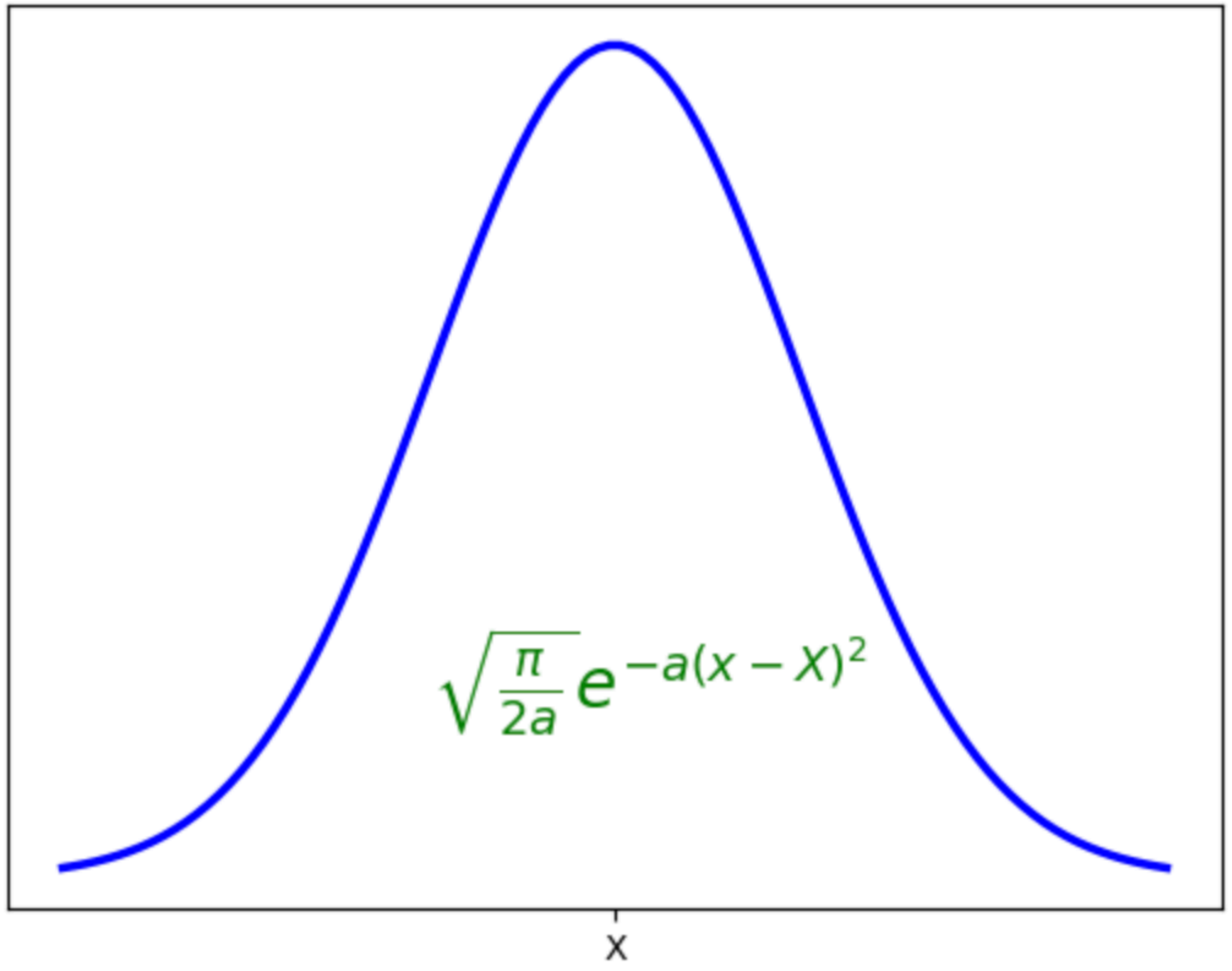
- The set of wave functions form a **vector space.** That is if $\psi_1(\mathbf{x}, t)$ and $\psi_2(\mathbf{x}, t)$ are both possible states of the system then so there is a linear combination: $\psi_3(\mathbf{x}, t) = \alpha\psi_2(\mathbf{x}, t) + \beta\psi_1(\mathbf{x}, t)$. With $\alpha, \beta \in \mathbf{C}$

- This is called the principle of superposition.

- Remember we are dealing with an infinite dimensional vector space. We don't consider any function, but only those that can be normalised.

Example

- Suppose that you have a particle that, at some time t_0, you know is localised somewhere near the point $\mathbf{X}$. We could describe as a Gaussian
- $\psi(\mathbf{x}) = \frac{1}{\sqrt{N}} e^{-a(x-\mathbf{X})^2}$
- a describe how spread out the wavefunction is.
- the probability distribution is not spread out over long distances, so the particle also retain something of its classical nature.

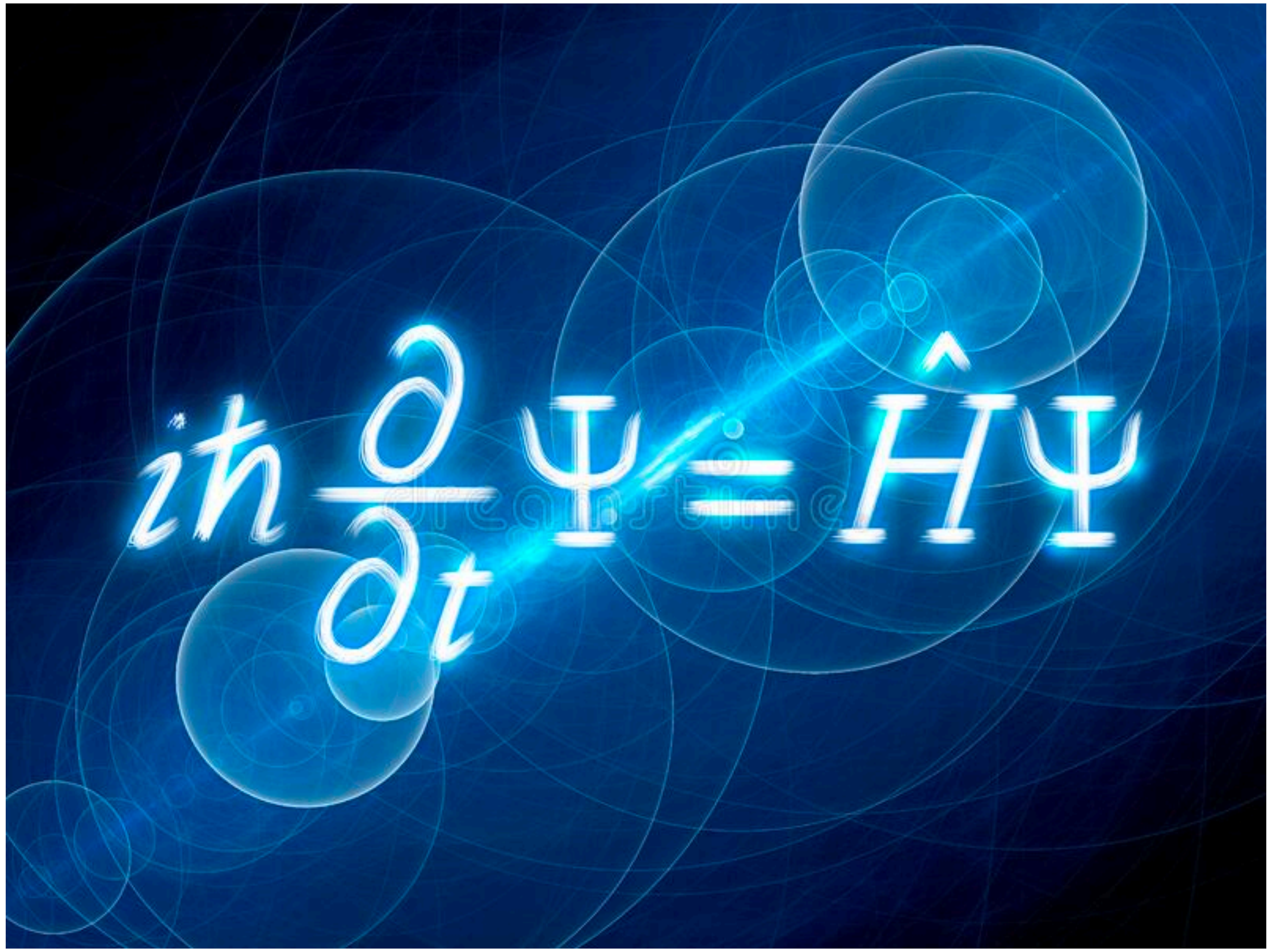


Example

- Superposition principle tells us that we should also entertain the idea that the particle can sit in a state:
- $$\psi(\mathbf{x}) = \frac{1}{\sqrt{N'}}\left(e^{-a(x-\mathbf{X_1})^2} + e^{-a(x-\mathbf{X_2})^2}\right)$$
- The interpretation of this state is that the particle has somehow split and now sits both near X1 and near X2.
- States like the one above, where elementary particles – which are, as far as we can tell, indivisible – are coaxed into travelling along two or more different paths simultaneously
- Paradoxical situations with cats that are both alive and dead.

The Schrodinger Equation

- Here $\hbar$ is Planck's constant, a fundamental constant of nature: $\hbar = 1.06 \times 10^{-34}$Js
- In quantum world the energy unit is electron volts (eV). 1 eV = 1.6×10^{-19} J
- The units that $\hbar$ carries are more important. It is similar to angular momentum. It is also the same dimension as the action in classical mechanics



The Hamiltonian

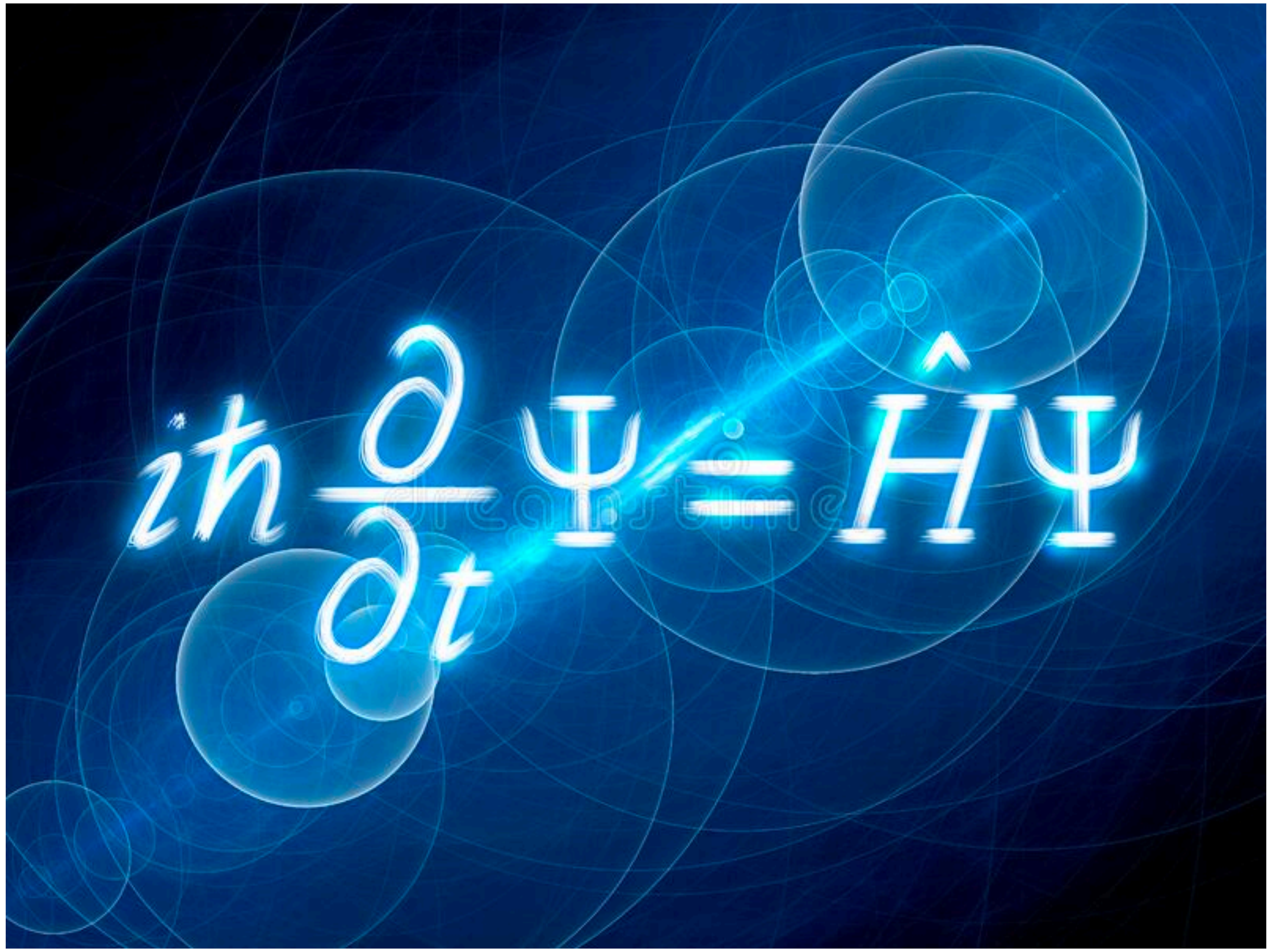
- The next thing in the Schrödinger equation is the Hamiltonian $\hat{H}$

- Different choices of Hamiltonian describe different laws of physics. We will use the example of non-relativistic particle moving in a potential.

- $$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})$$

- This is an example of a differential operator. The laplacian is defined by

- $$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$



The Hamiltonian

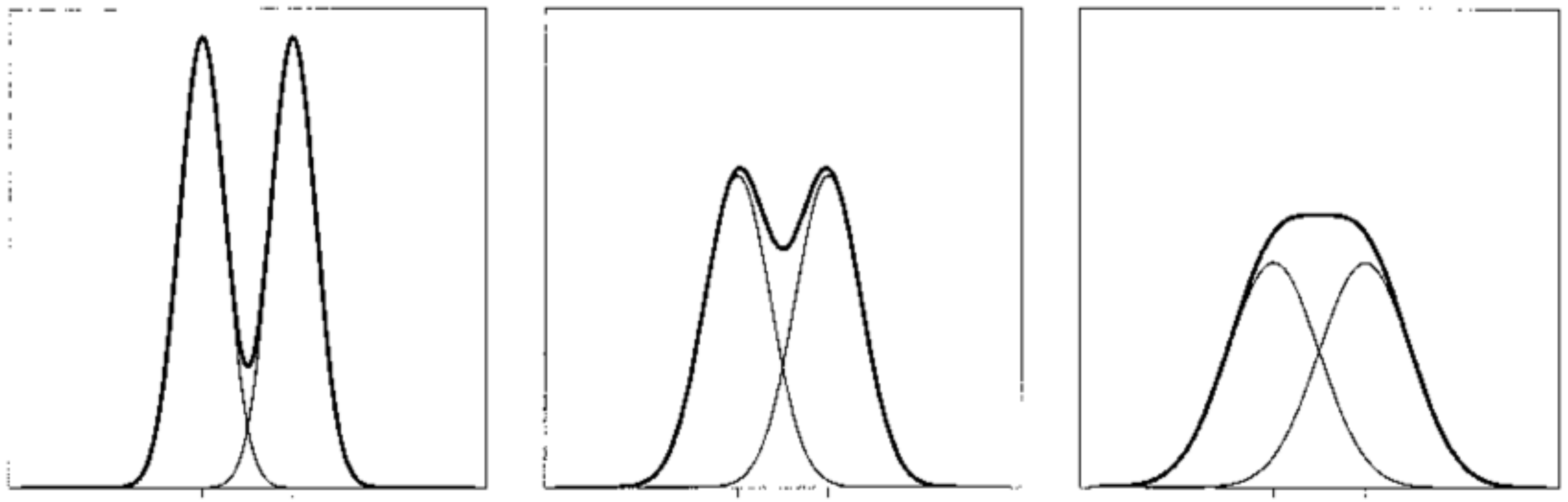
- Th “Hamiltonian” is not something entirely novel to quantum physics.
- In classical dynamics, the hamiltonian represents the energy of the system (kinetics + potential)
- If Hamiltonian operator in qm and classical dynamics have the same meaning does it mean that, $p \to \pm \hbar\nabla$?
- The energy only depends on p^2. How could the momentum of a particle – which, after all, is just a number — possibly be related to something as abstract as taking a derivative?
- Not all classical theories can be written using a Hamiltonian. Only those theories that have **conservation of energy** can be formulated in this way. Importantly, the same is true of quantum mechanics

- In many ways that's no big loss.
- The friction forces that dominate our world are not fundamental, but the result of interactions between many (say 10^{23}) atoms.
- There are no such friction forces in the atomic and subatomic worlds and, moreover, the formalism of quantum mechanics does not allow us to easily incorporate such forces

If, for some reason, you really do want to consider quantum friction then you're obliged to include the direct coupling to the 10^{23} other atoms and track what happens. There are interesting applications of this, not least an idea known as decoherence.)

Collapse of the Wavefunction

- In only one way the Schrodinger equation does not describe the evolution of a quantum state. This occurs when we do a **measurement.**

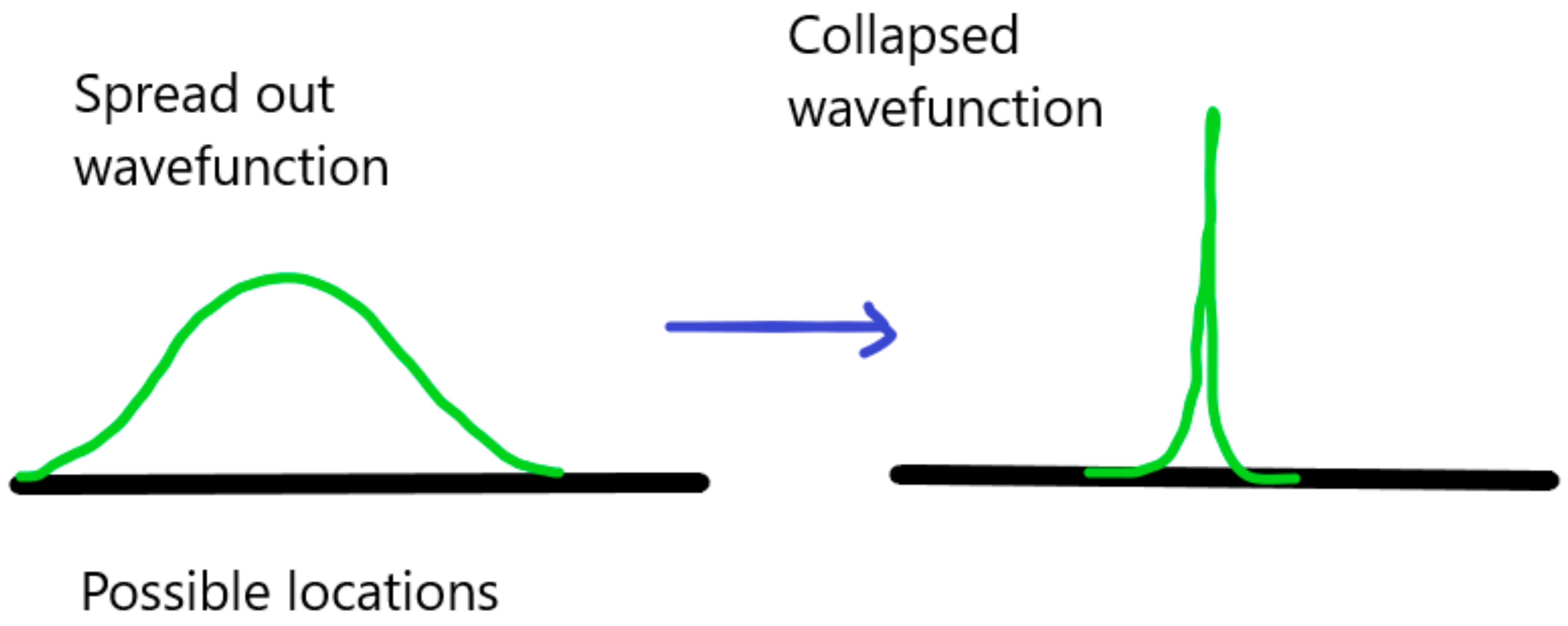


- $$\psi(\mathbf{x}, t_0) = \frac{1}{\sqrt{N'}}\left(e^{-a(x-\mathbf{X_1})^2} + e^{-a(x-\mathbf{X_2})^2}\right)$$

- Let's say we do a measurement using a detector. We place a detector at X1 and detect the presence of the particle there. This means that the probability density at X2 vanish

- After the measurement:

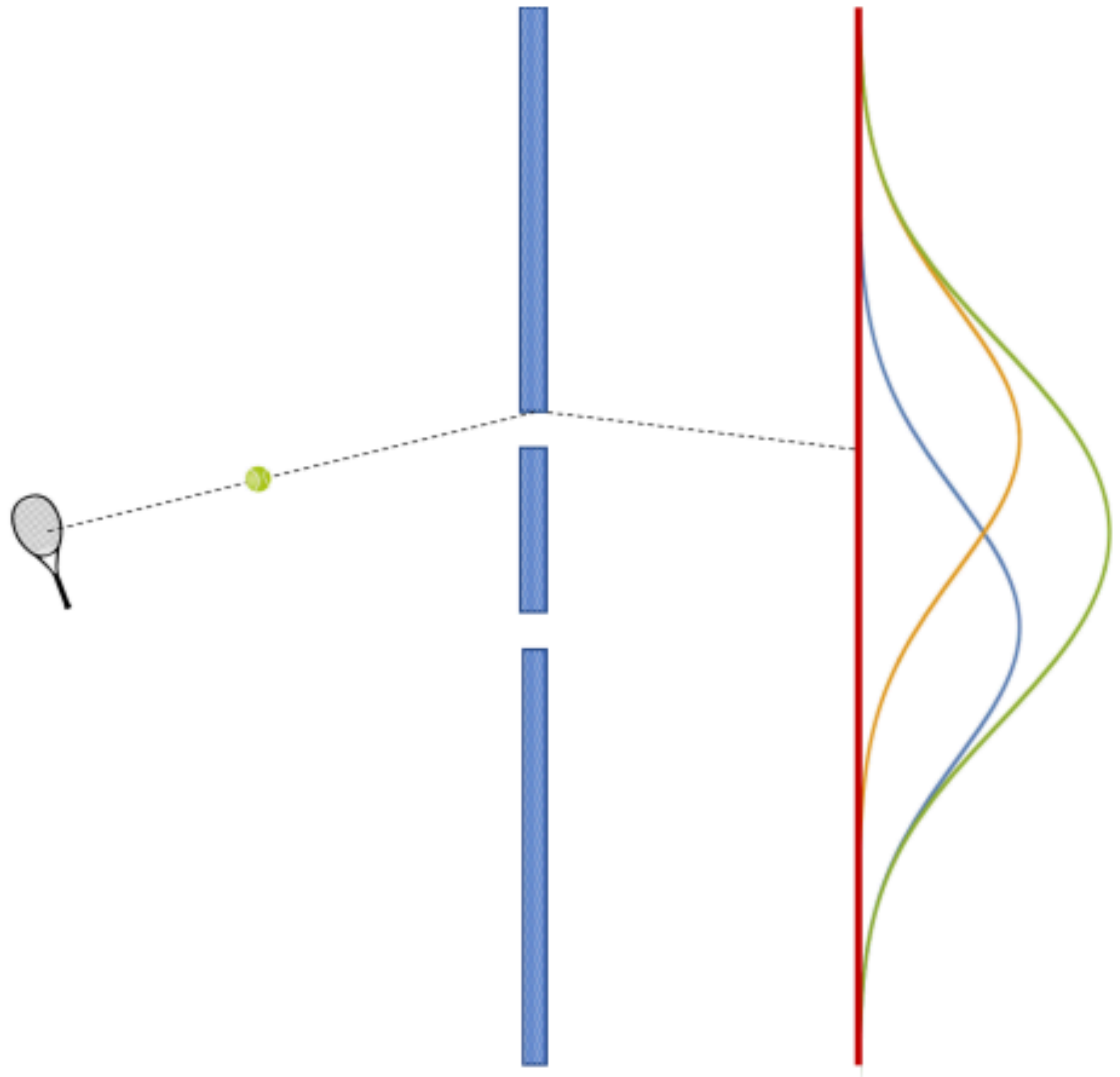
$$\psi(\mathbf{x}, t_+) = \frac{1}{\sqrt{N}}e^{-a(x-\mathbf{X_1})^2}$$



- The fact that the wavefunction can evolve in two very different ways – the first through the smooth development of the Schrodinger equation, the second from the abrupt collapse after measurement – is one of the most unsettling aspects of quantum mechanics.

Double slit experiment

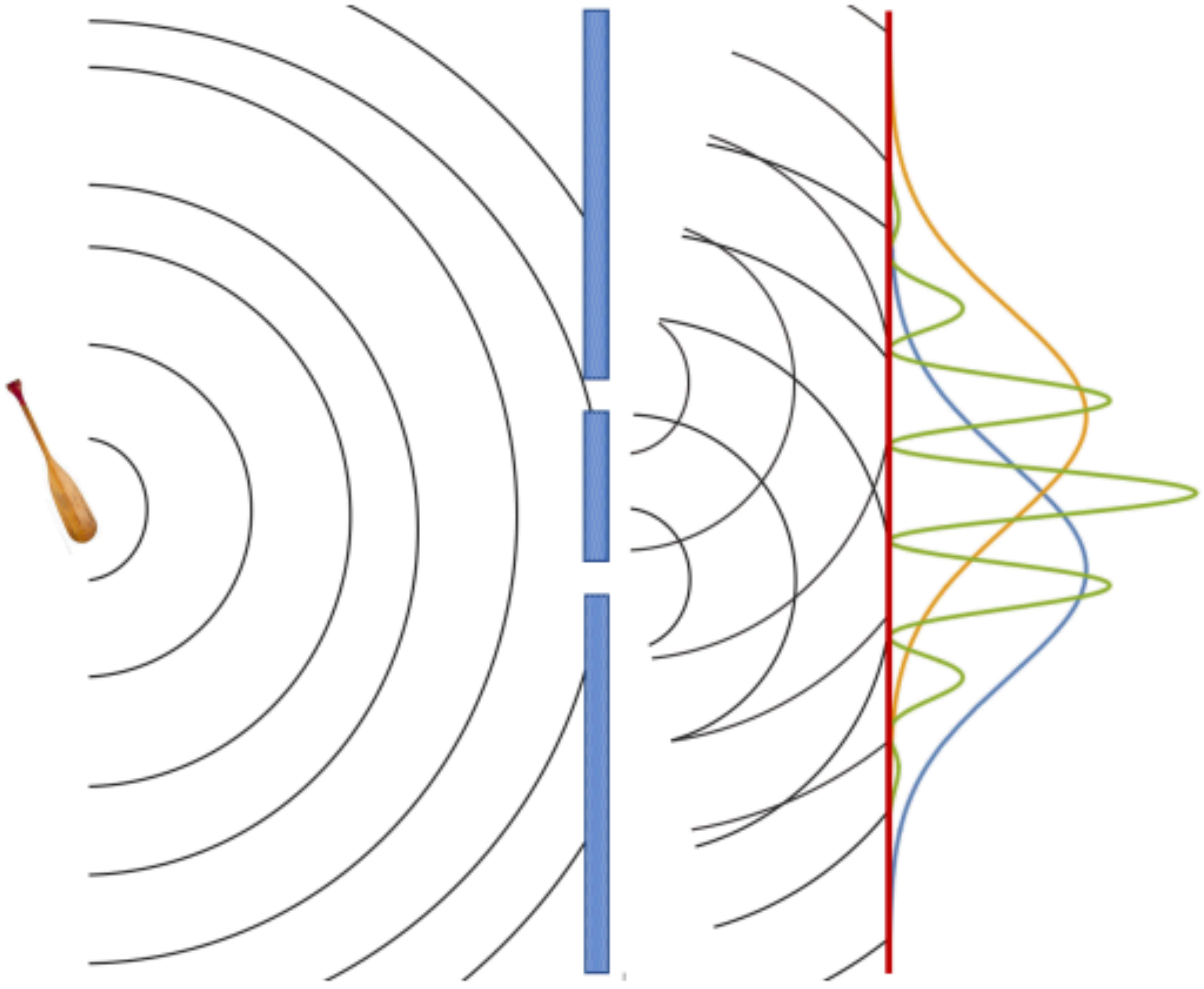
- $P_{12} = P_1 + P_2$



The distribution of the classical particle

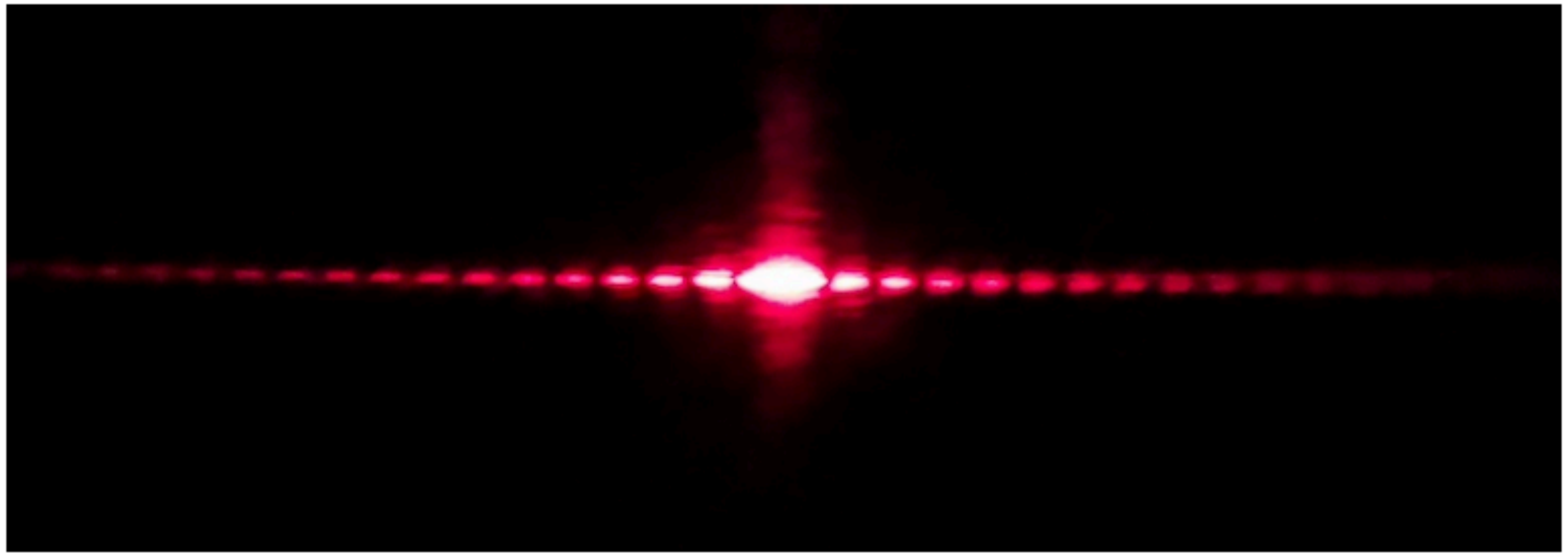
Double slit experiment

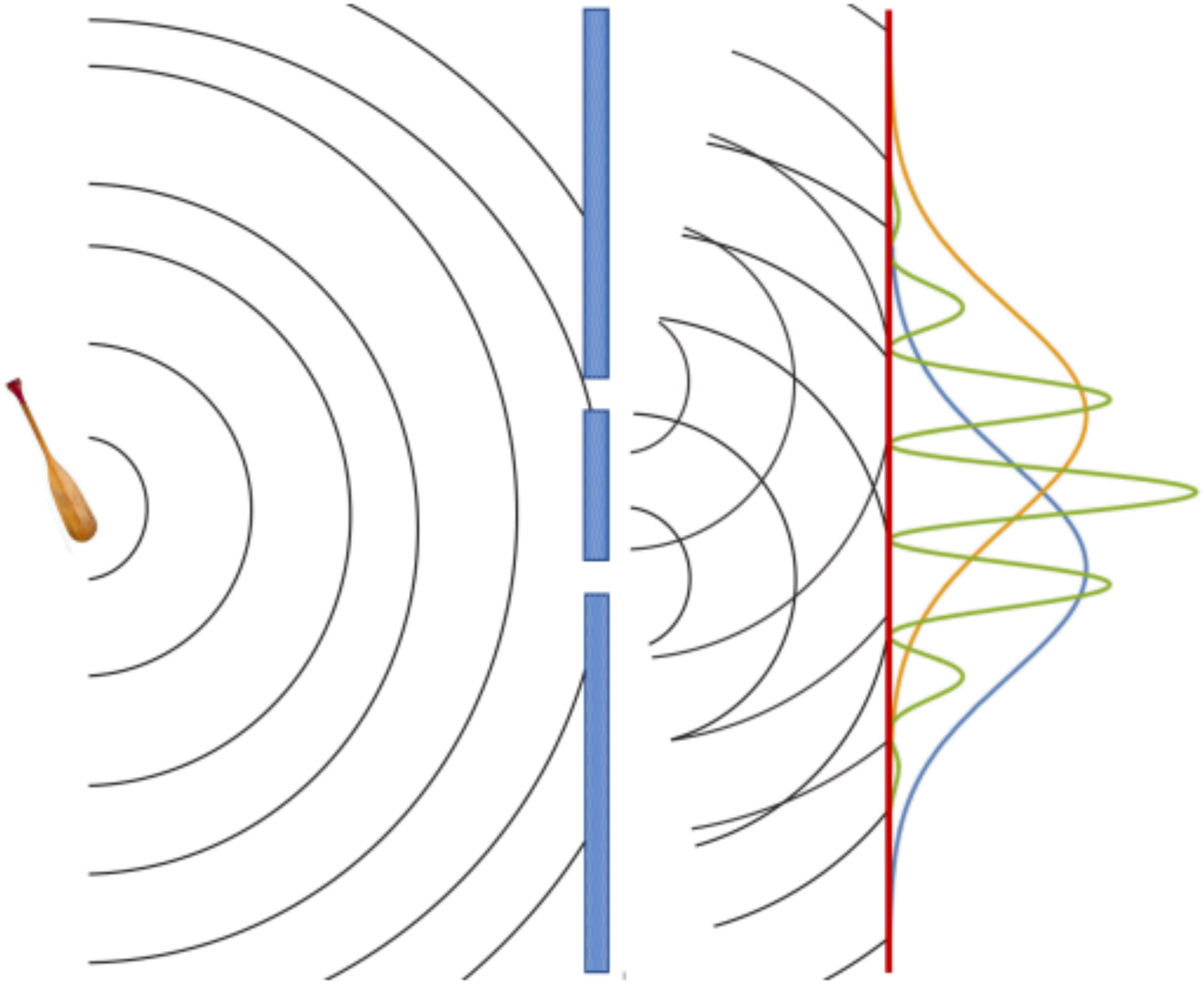
- For any kind of wave, there is a new ingredient that dramatically changes the outcome: this is interference
- The end result is very similar to that of a particle: a distribution spread out, peaked around the position of the first slit.
- The real difference comes when we open both slits. The waves pass through along two paths and, when they recombine on the other side, add constructively or destructively.



The distribution of the classical waves

Double slit experiment





The distribution of the classical waves

Double slit experiment in quantum world

- Electrons
- For appropriately sized slits, the result is a combination of the two classical experiments described above.
- First, when we detect an electron it appears just like a classical particle would appear
- After playing the game many times, the probability distribution seen on the screen agrees with that of a classical wave, exhibiting an interference pattern.
- **The most striking aspect of this result** is that there are certain places on the screen where fewer electrons are detected when both slits are open than when any one slit is open
- Particle somehow knows about the presence of both slits.

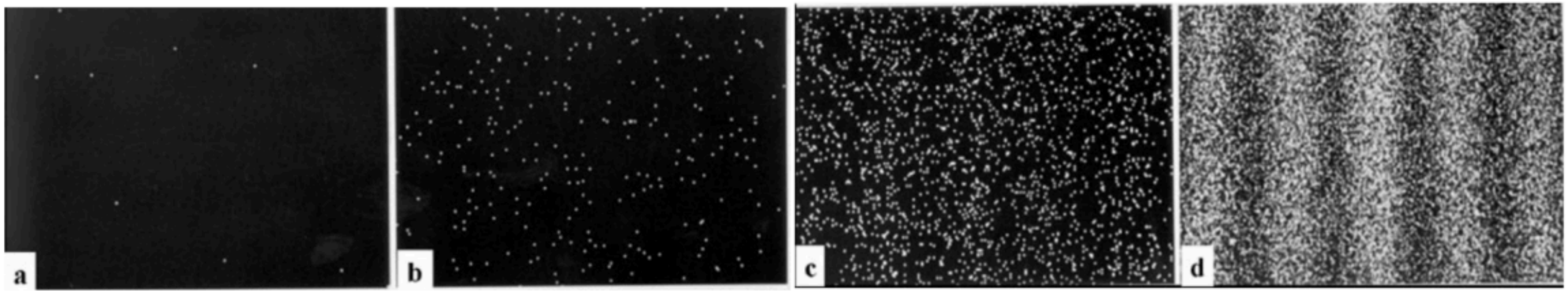


Figure 5. The double slit experiment, performed by Hitachi. The results show the build up the interference pattern from 8 electrons, to 270 electrons, to 2000 electrons and, finally, to 160,000 electrons where the interference fringes are clearly visible.

- $P_1 = |\psi(x)|^2$
- $P_{12} = |\psi_1(x) + \psi_2(x)|^2 = P_1 + P_2 +$ cross terms
- These cross terms are responsible for interference pattern