Simulation 1: Schrödinger Eqn.

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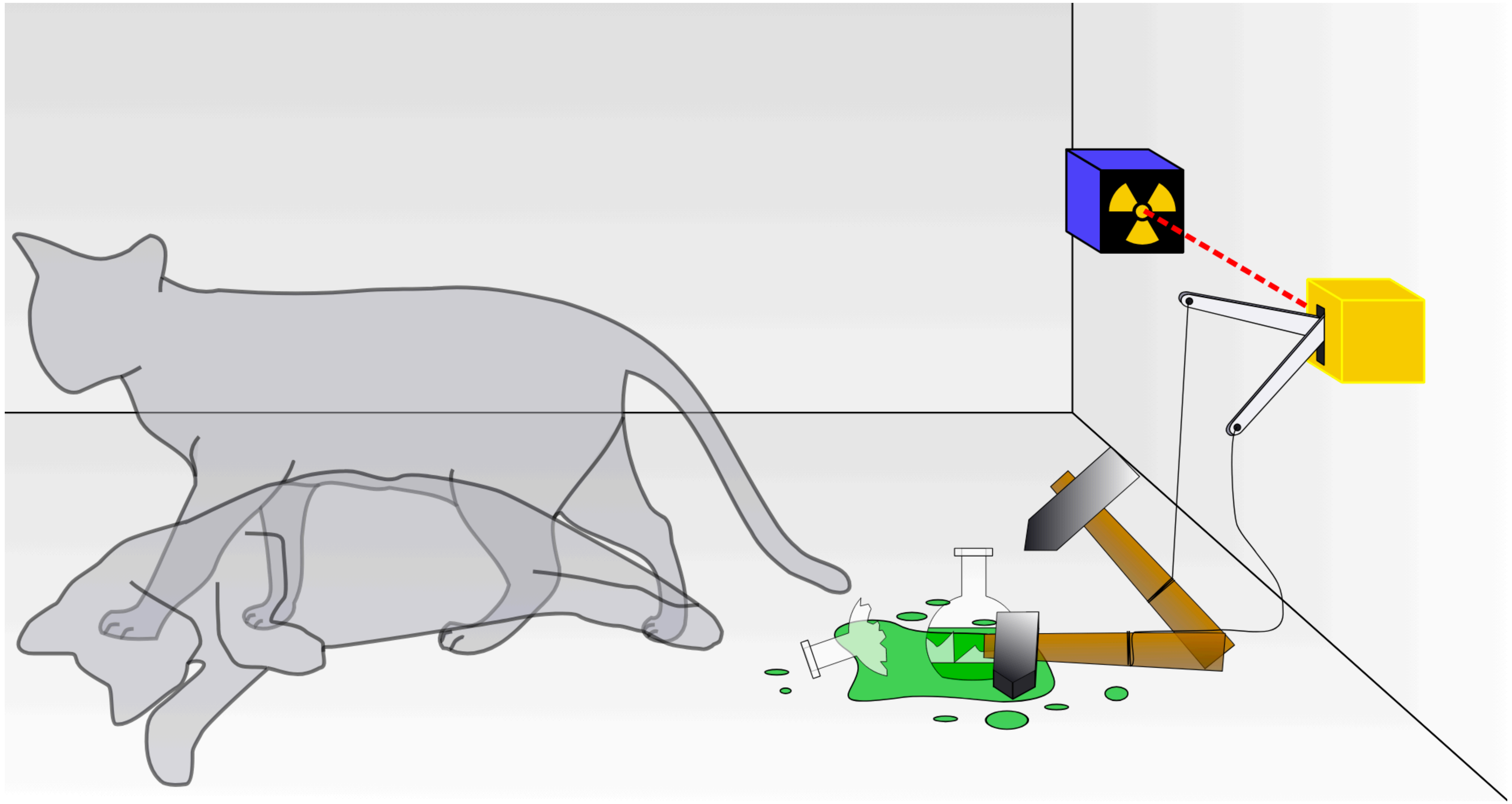
27 July 2023

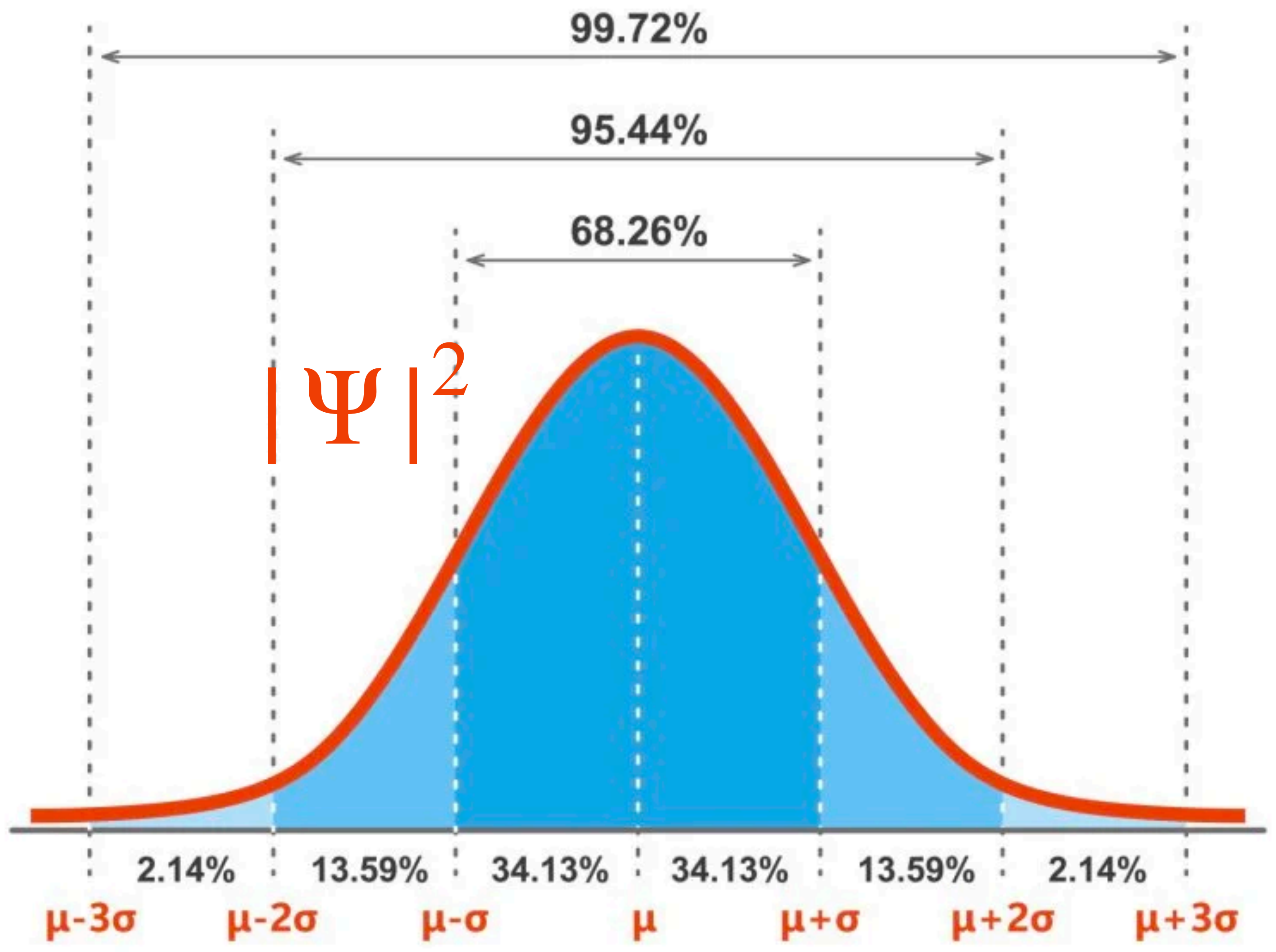
Schrödinger's cat

- We have discussed already Schrödinger's cat, the thought experiment in which a vial of poison is released if a radioactive isotope decays.
- It's said that the cat is both alive and dead until the box is opened. Before opening the cat is in a "quantum superposition" of both dead and alive.
- But why?



Schrödinger's quantum wave equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\Psi$$



- **The Schrödinger Equation describes the quantum wave function of particles.**

- **Particles do not have a position until it is measured. The square of the wave function tells you the probability of finding the particle in some region**

- **The constant $\hbar$ is the quantization of energy. Energy comes in packets of $\hbar$. It is the "step size" on the energy ladder**

- **Note the use of imaginary numbers! $|\Psi|^2$ is the amplitude of a complex number: $|a+ib|^2 = \sqrt{a^2+b^2}$. Imaginary numbers "are not real" but they are critical to our most accurate theories of reality!!**

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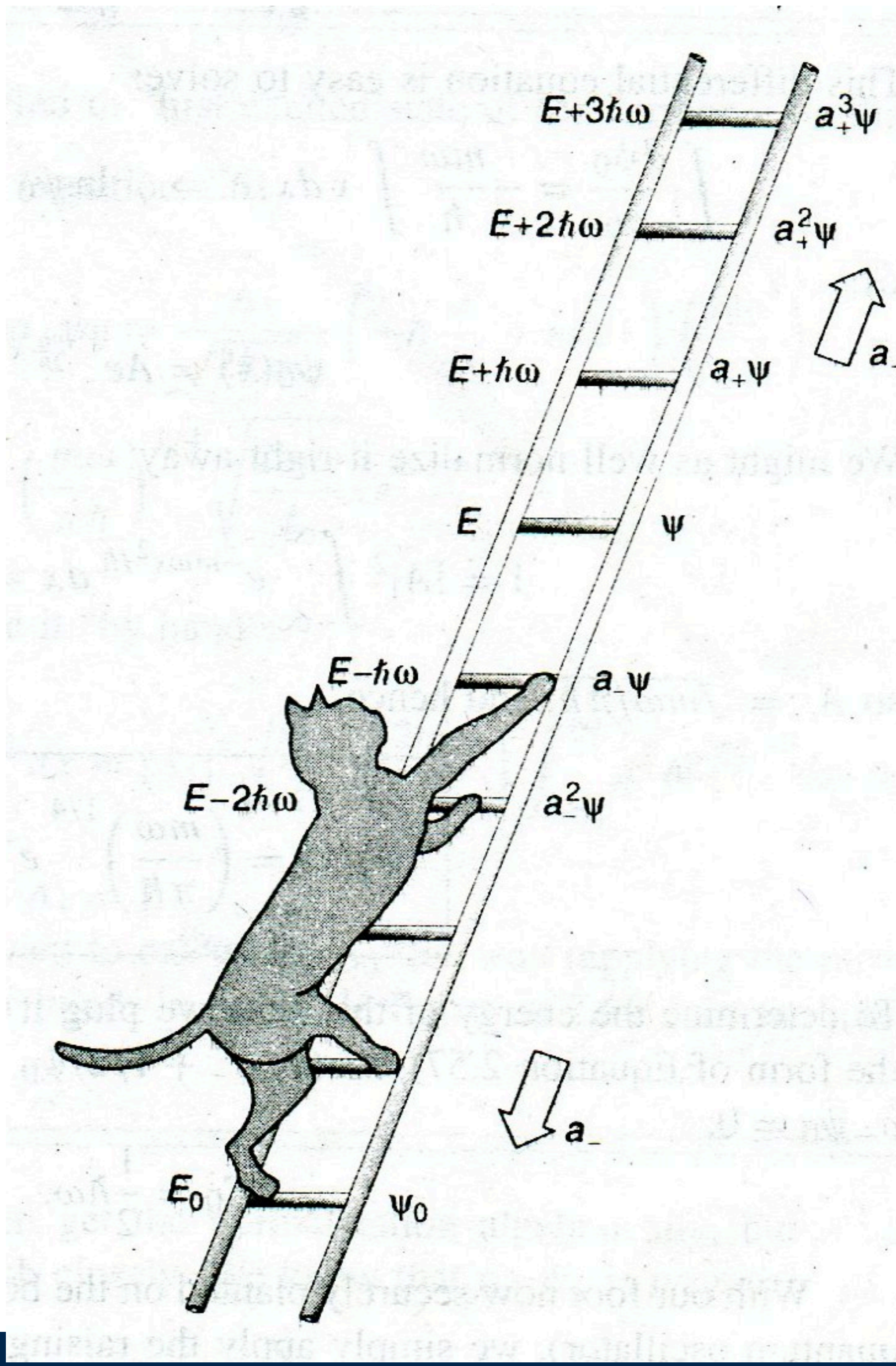
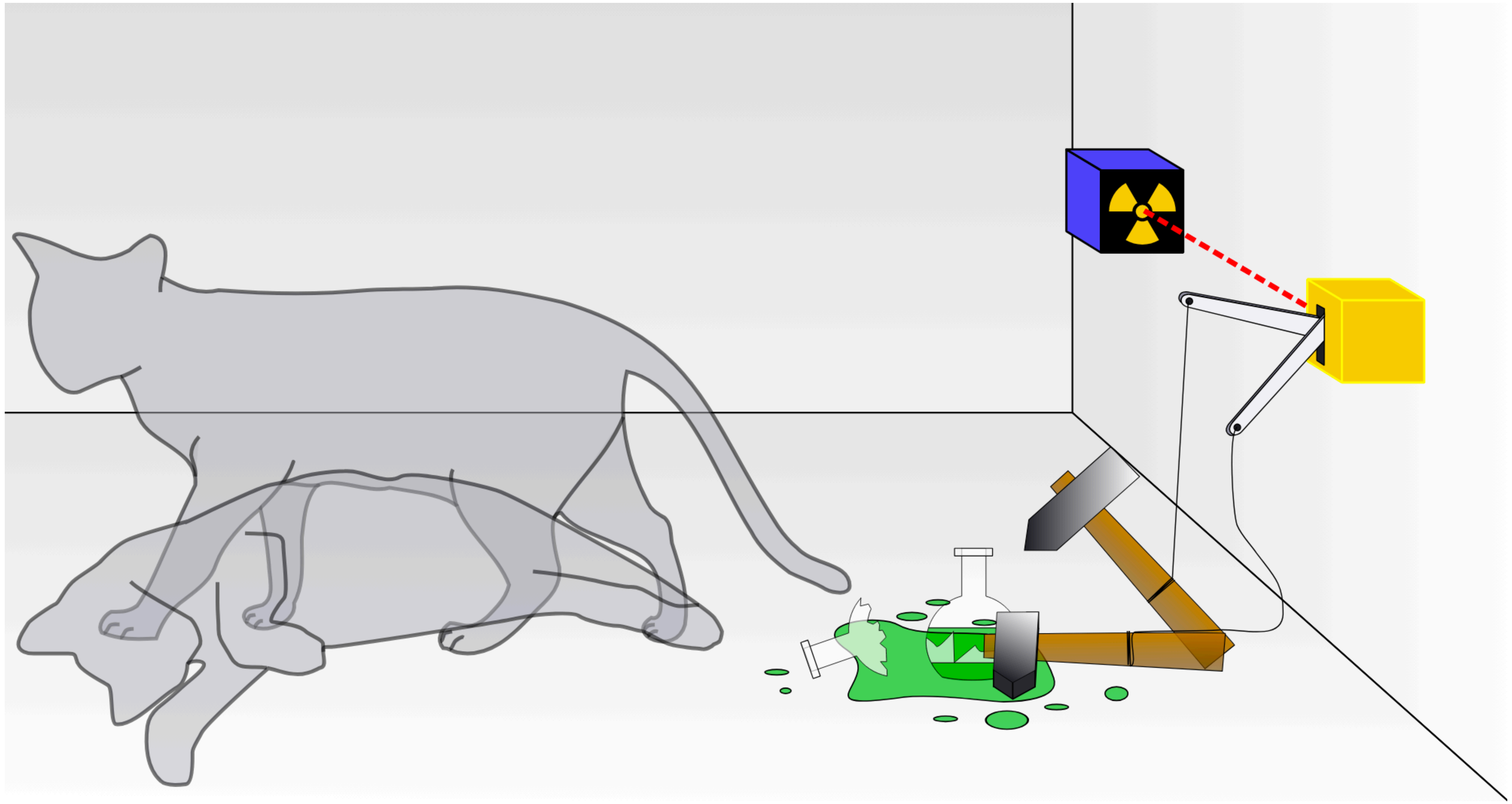


Schrödinger's cat

- **So, because the radioactive isotope has a *probability* of decaying, we can't know for sure whether it does until we open the box.**

- **Schrödinger originally proposed the thought experiment to highlight the absurdity of quantum superposition, and it remains controversial in interpretation to this day.**



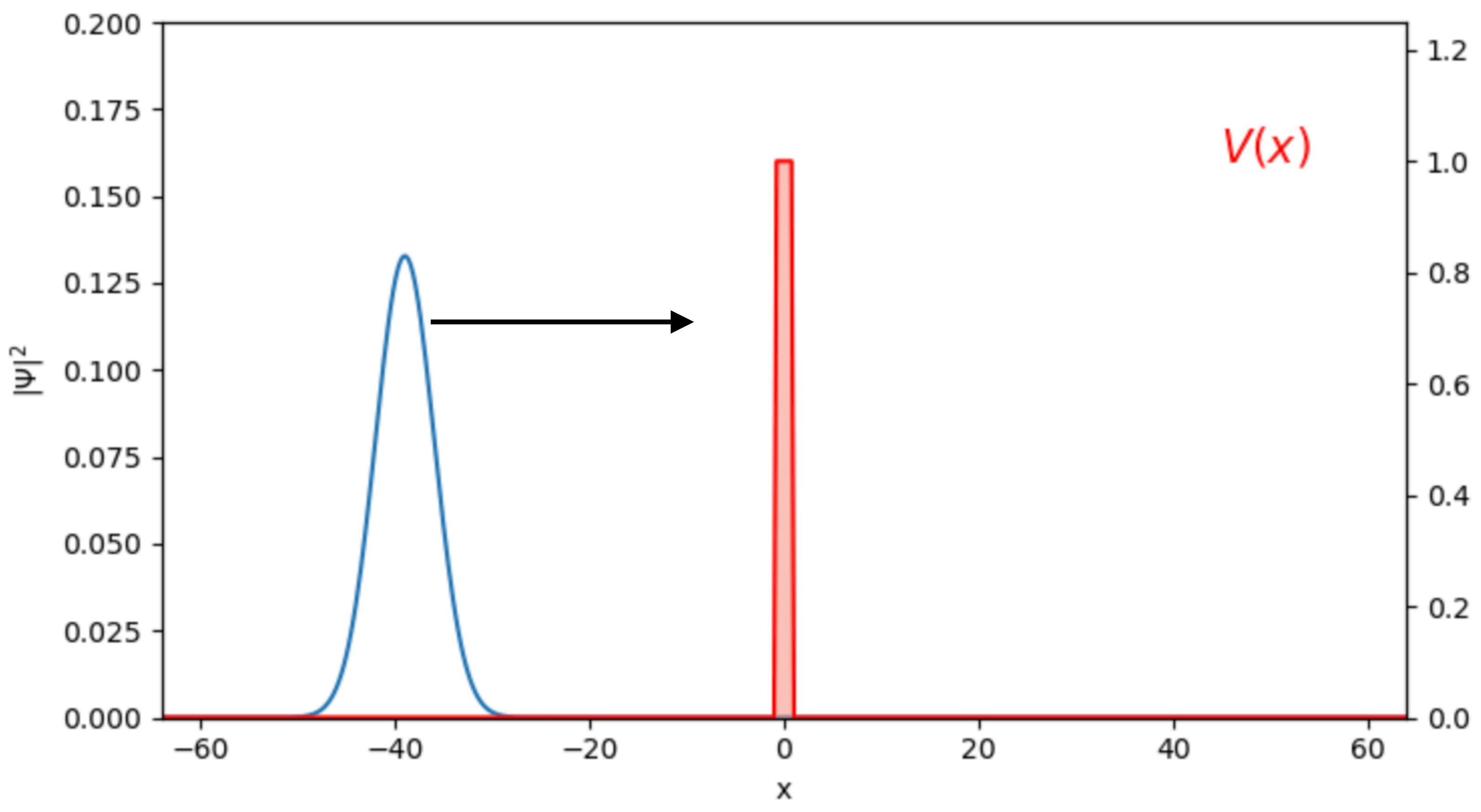
Quantum Tunneling

- **Imagine we have a quantum wave packet moving to the right towards an energy barrier.**
  - The wave packet has half as much energy as the energy barrier.
  - What happens?

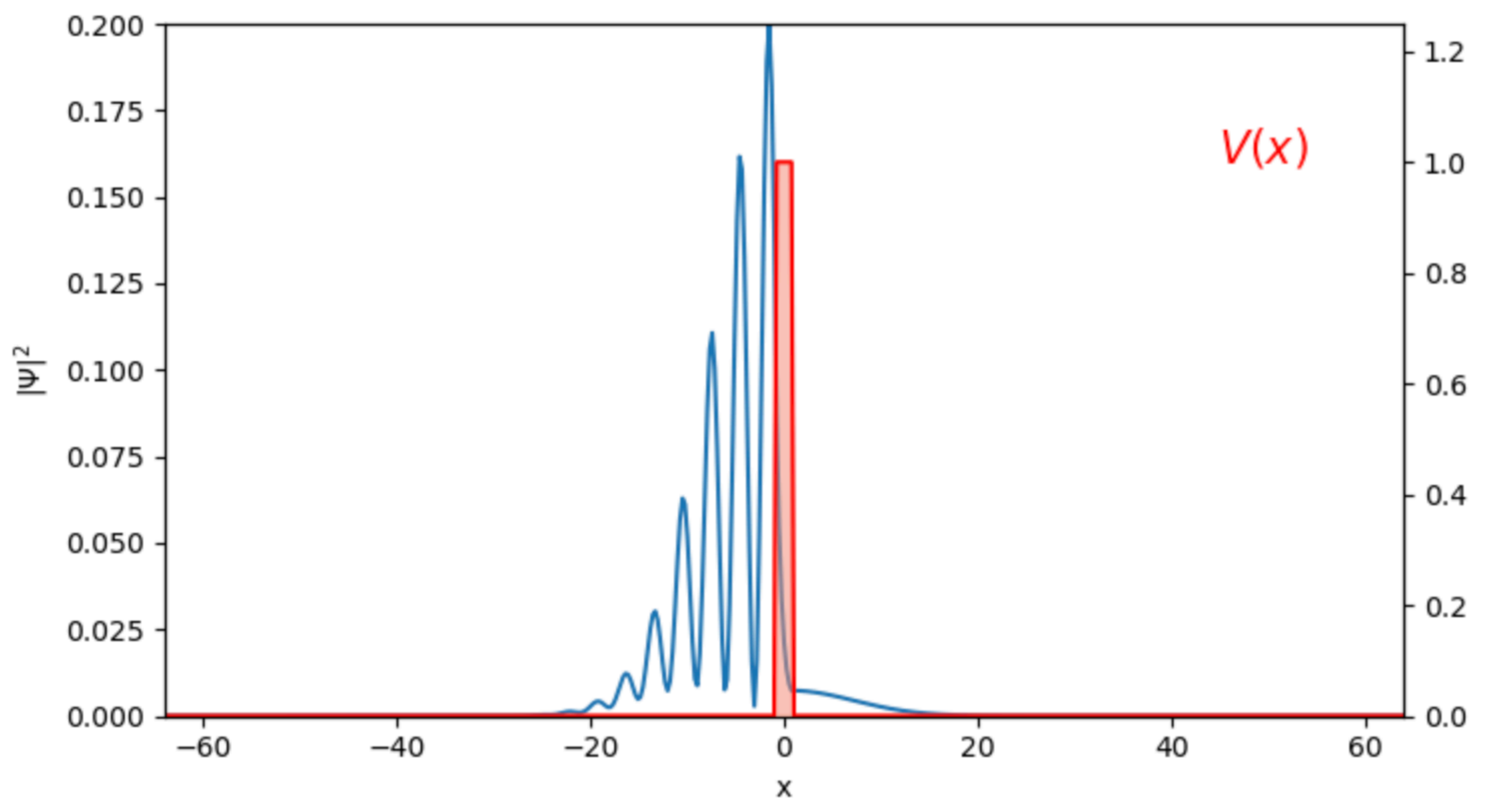
- **In classical physics, the packet bounces off the barrier and starts moving to the left.**

- **In quantum physics, this happens *and* some of the wave function leaks through to the right.**

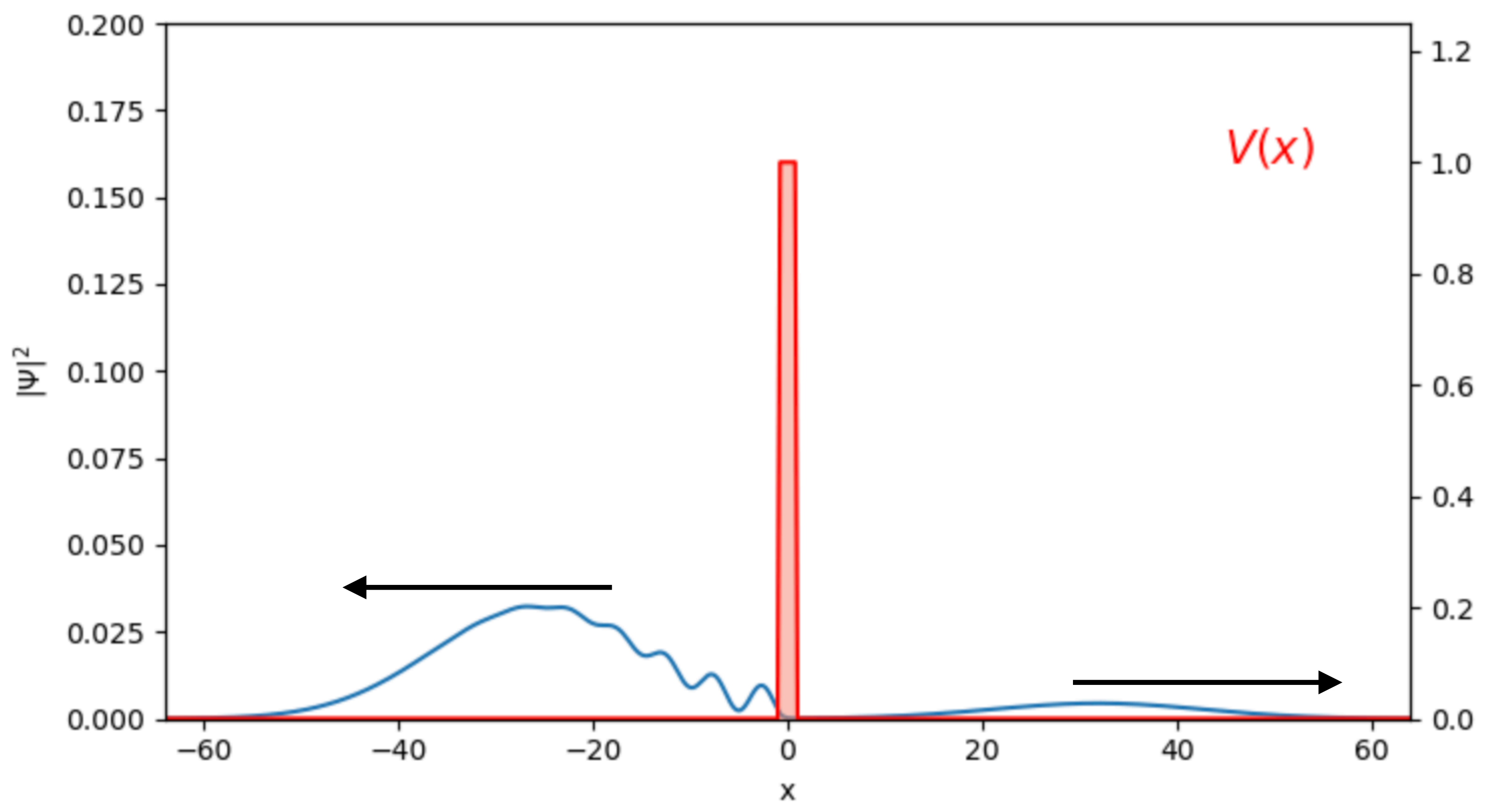
- **We don’t know if the particle bounced off the barrier or tunneled through it until we “open the box”**



$t = 0$



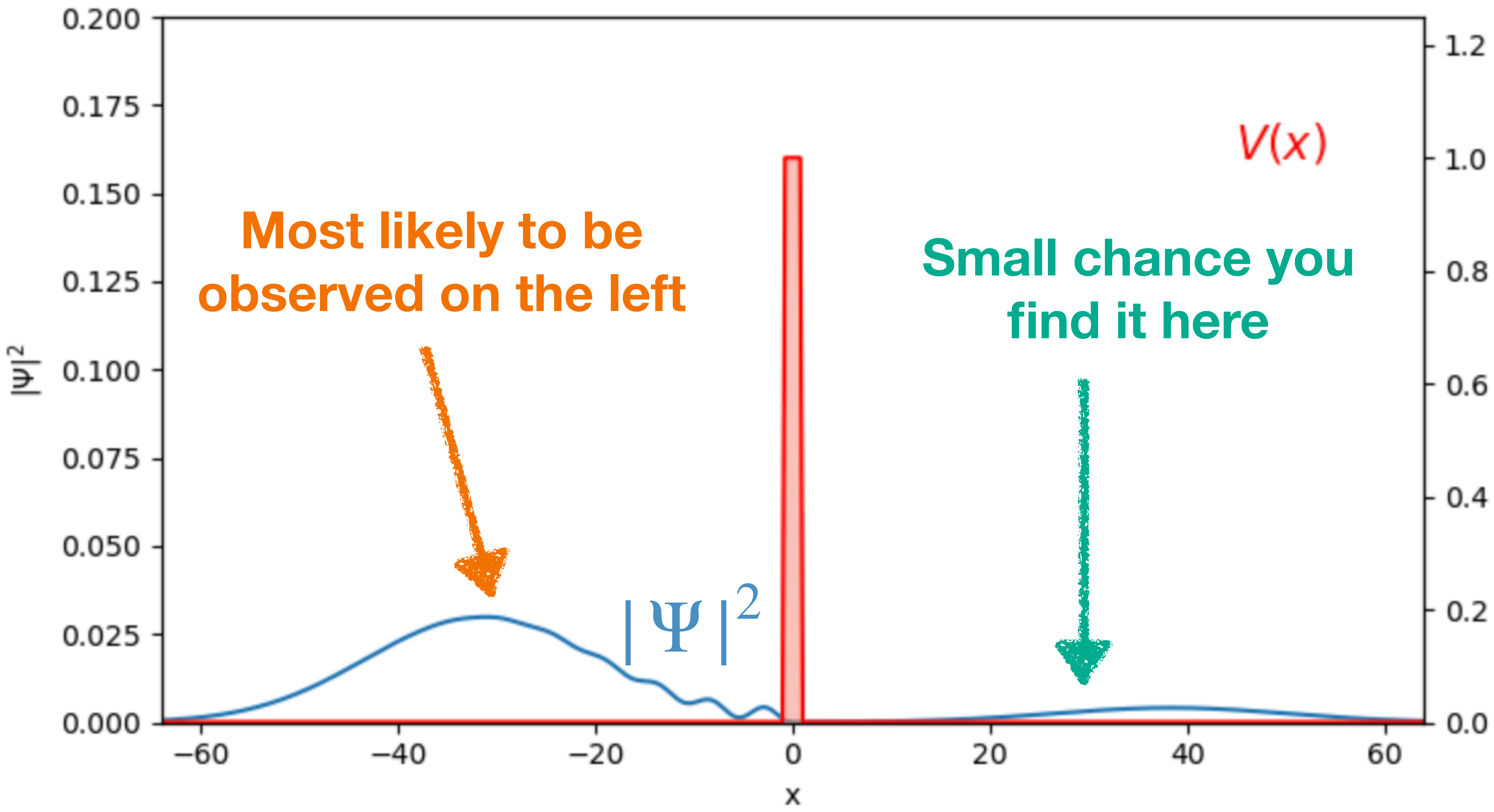
$t = 1$



$t = 2$

What if we open the box?

- We are not simulating wave function collapse, but simply the evolution of the quantum wave function.
- If you pause your simulation at a given time, the function currently displayed shows the probability of the particle to be in any particular location (we square the wave function before plotting it)
- When you "open the box" you just get the position of the particle. In this case the most likely answer is x=-30, but you could sometimes get x=-20 or -50. If you repeat the experiment rarely, but sometimes, you'll get a positive number.
- When you open the box in Schrödinger's thought experiment, you find out if the cat is alive or dead. It will be one or the other, not both.



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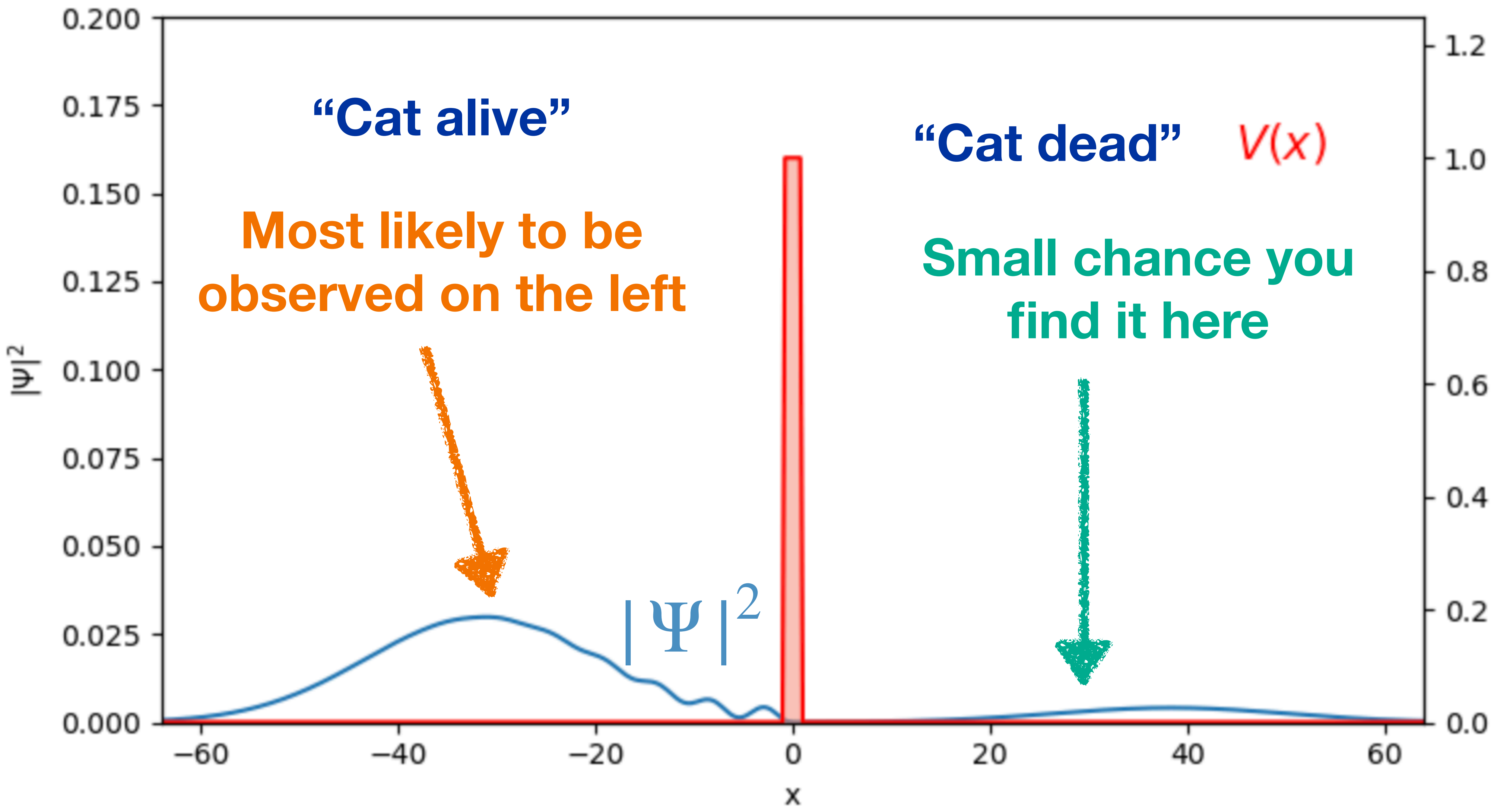

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- **The Schrödinger Equation is a *differential equation*. It is an equation with derivatives of functions inside it.**

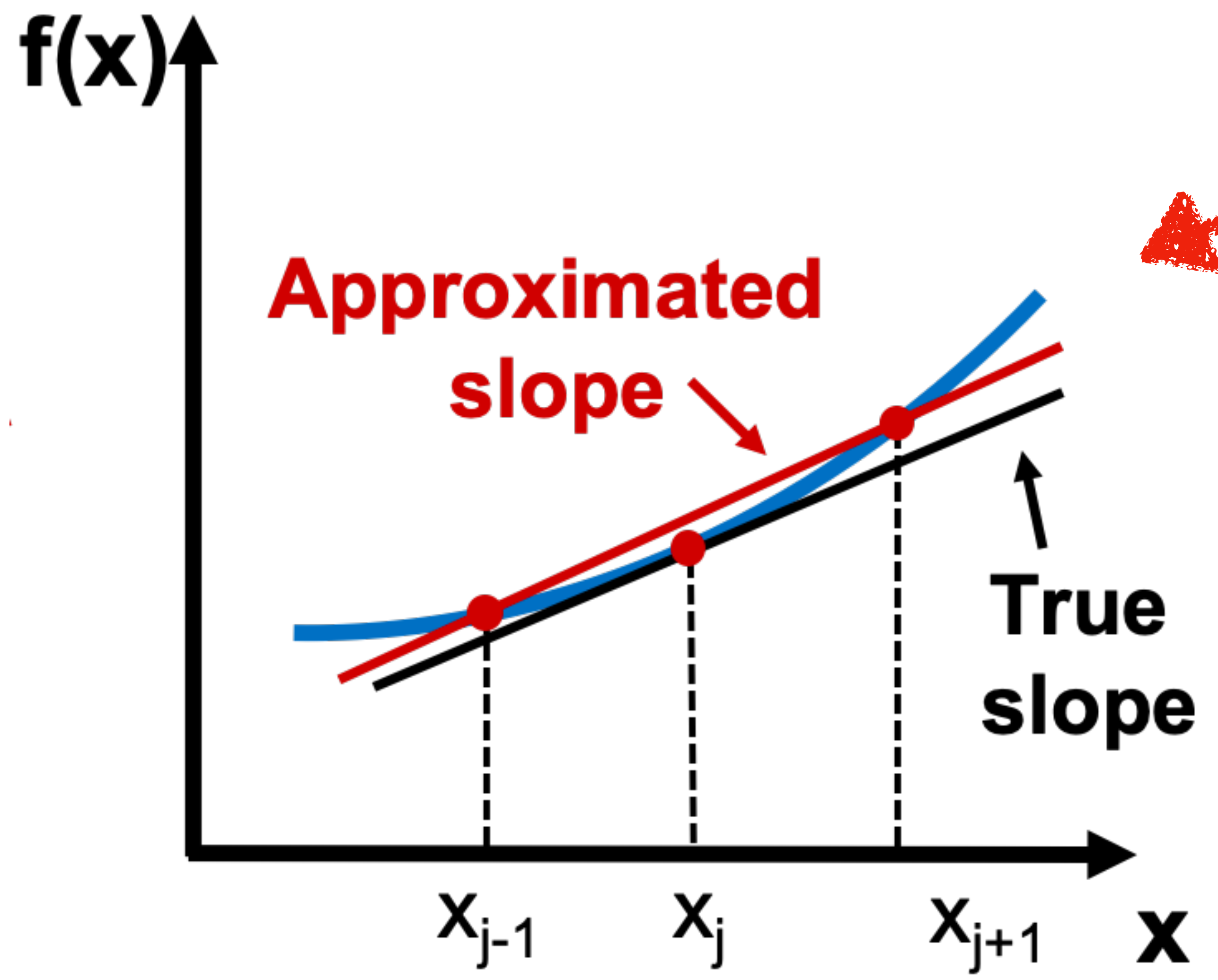
- **Differential equations are *everywhere* in physics:**
  - Newtonian physics: $F = ma = m\frac{d^2x}{dt^2} = \frac{dp}{dt}$
  - Fluid dynamics
  - Schrödinger equation and other quantum wave equations

- **Once we have an initial state, we can use this equation in a computer simulation to tell us what the function will look like after some small time step Δt.**

Today's Simulation

- **Today you will run a numerical simulation of the Schrödinger Equation to learn about its strange properties**
  - Quantization of energy
  - Quantum tunneling
  - Self-interference and wave-particle duality

- **The simulation uses approximations of derivatives by discretizing space and time**



Derivatives are hard

$$i\hbar \boxed{\frac{\partial \Psi}{\partial t}} = \frac{-\hbar^2}{2m} \boxed{\frac{\partial^2 \Psi}{\partial x^2}}$$

Approximate them by Evaluating the function At two nearby points

$$\frac{\partial f}{\partial x} \approx \frac{f(x+h) - f(x)}{h}$$

- **The numerical simulation will be in the form of a *Jupyter notebook*. Running the notebook will require you to write small amounts of python code. The simulation has already been written.**

Kevin Nelson