Simulation 1: Schrödinger Eqn.

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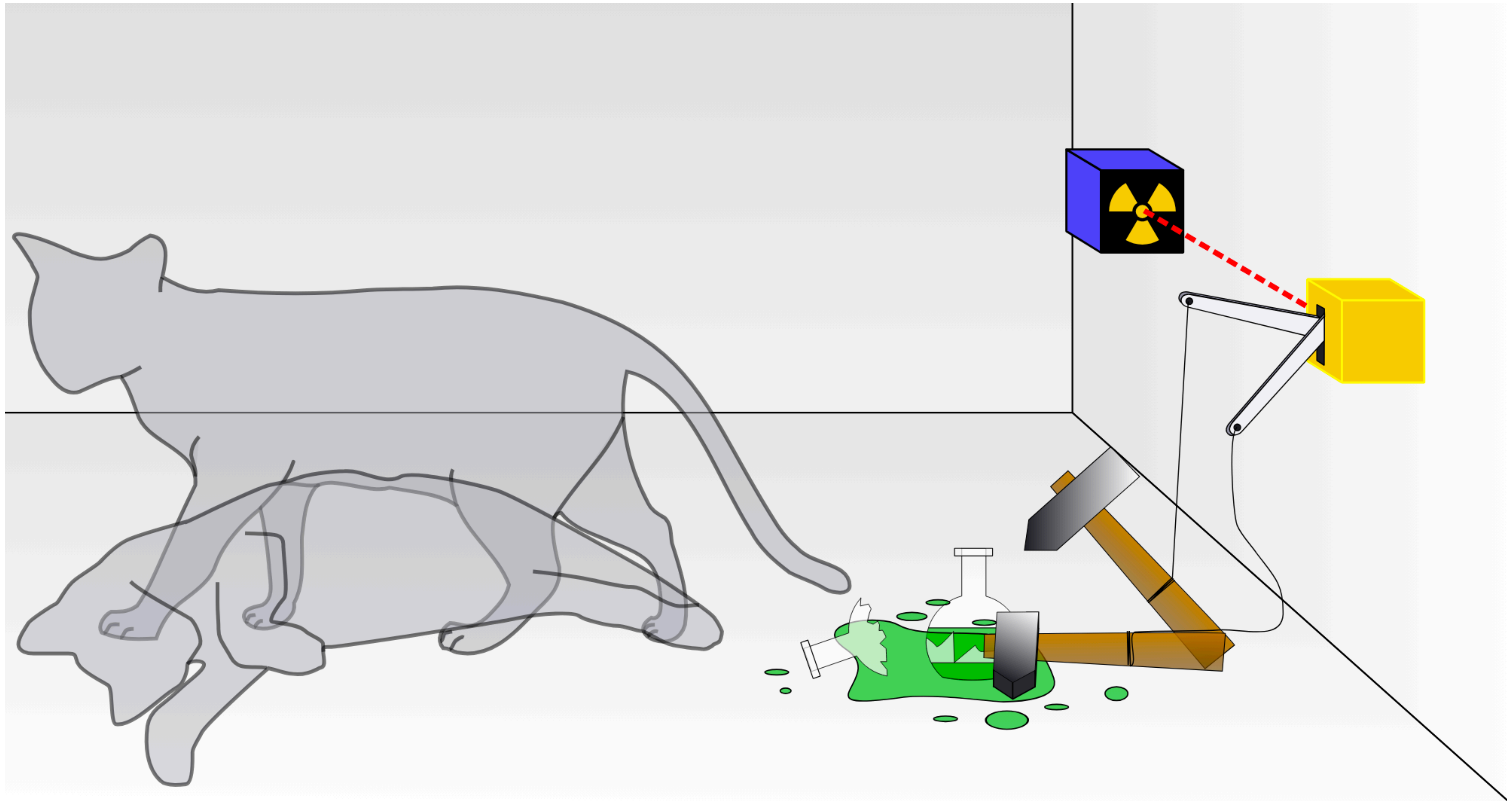
Schrödinger's cat

- You may be familiar with 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?



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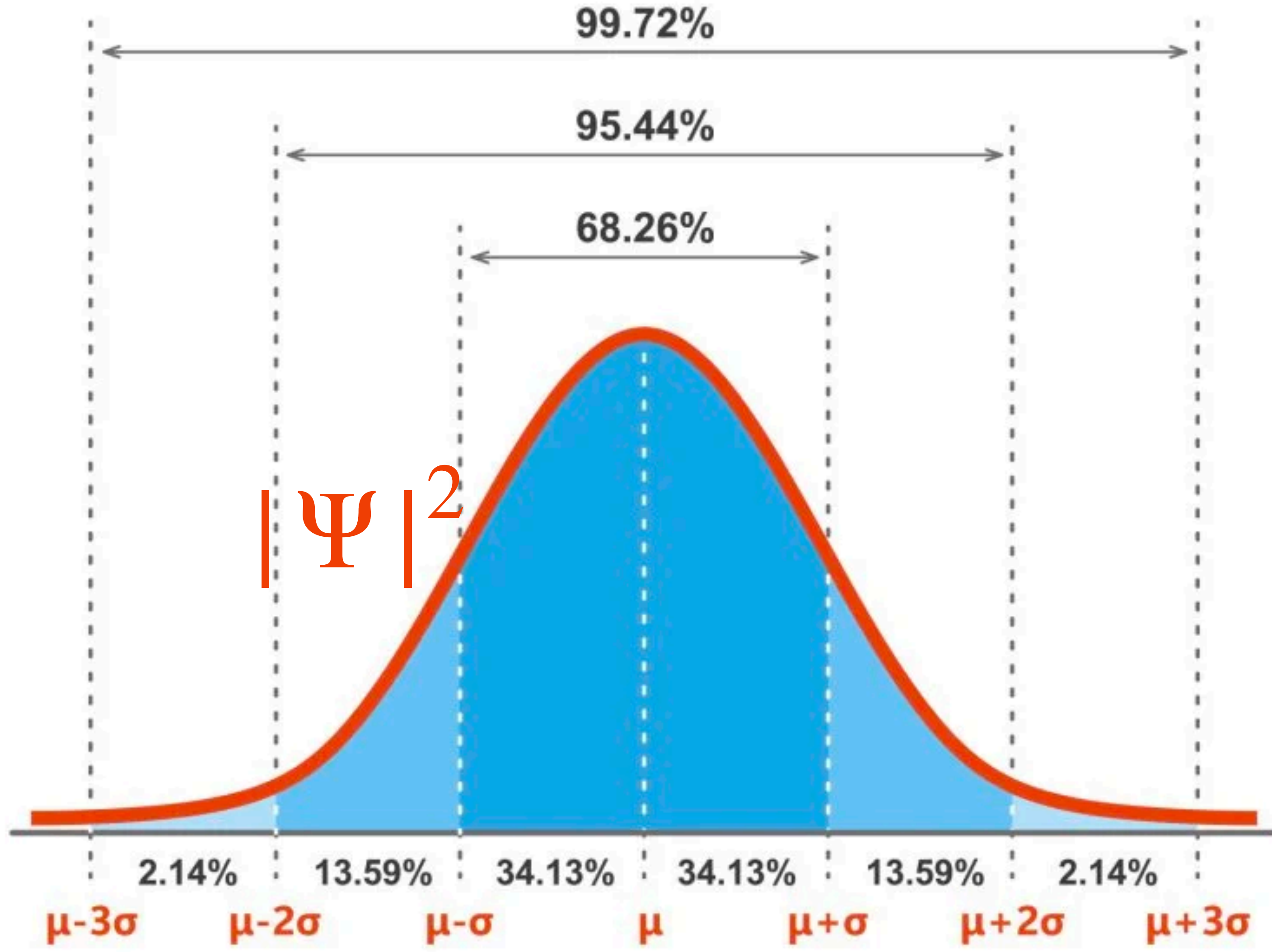
- **Particles do not have a position until it is measured. The square of the wave function tells you the probability of finding the particle in some region**



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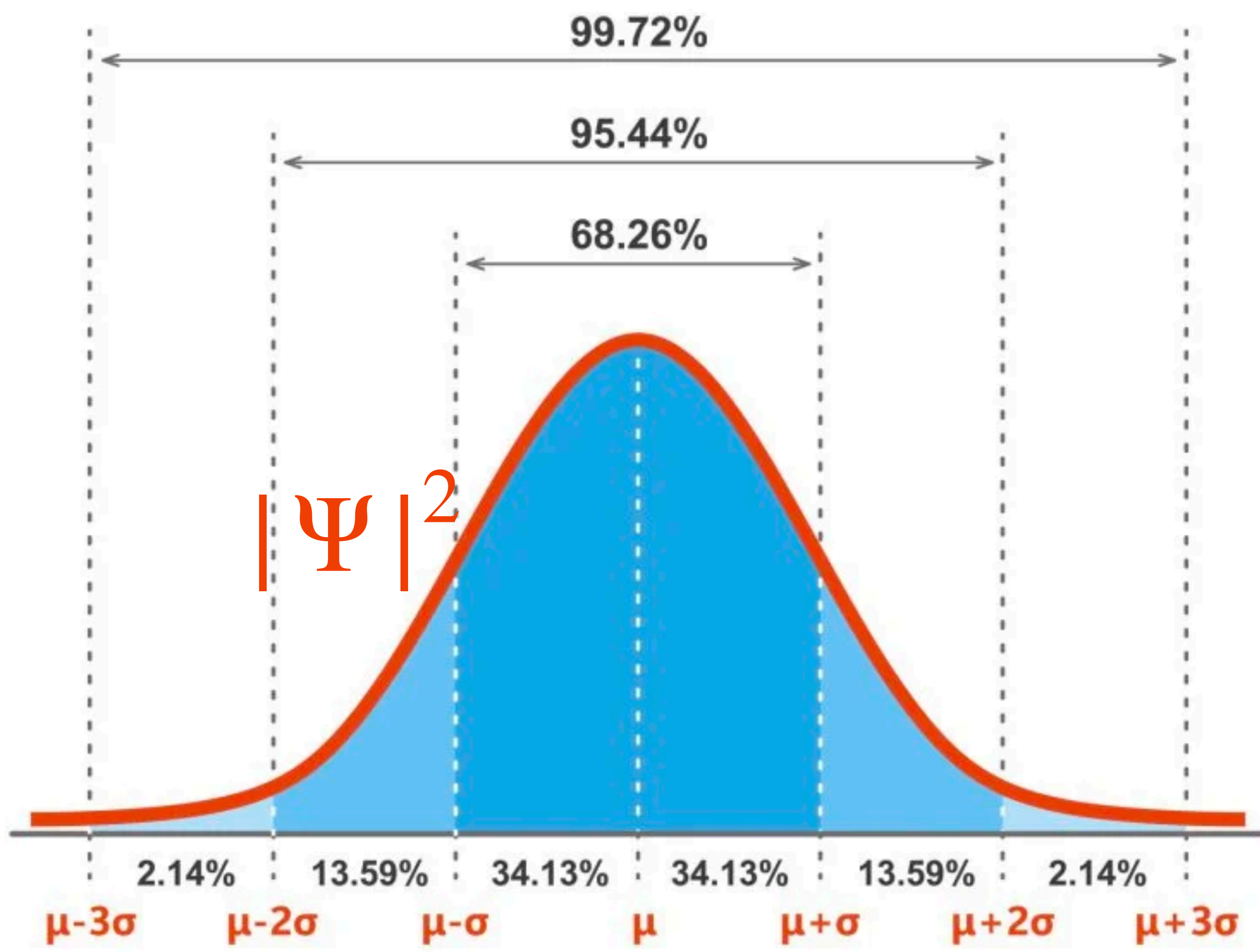
- **The constant $\hbar$ is the smallest possible value of energy. Energy is quantized into tiny packets. You can have 0, $\hbar$, 2$\hbar$,… but not 0.13$\hbar$ units of energy**



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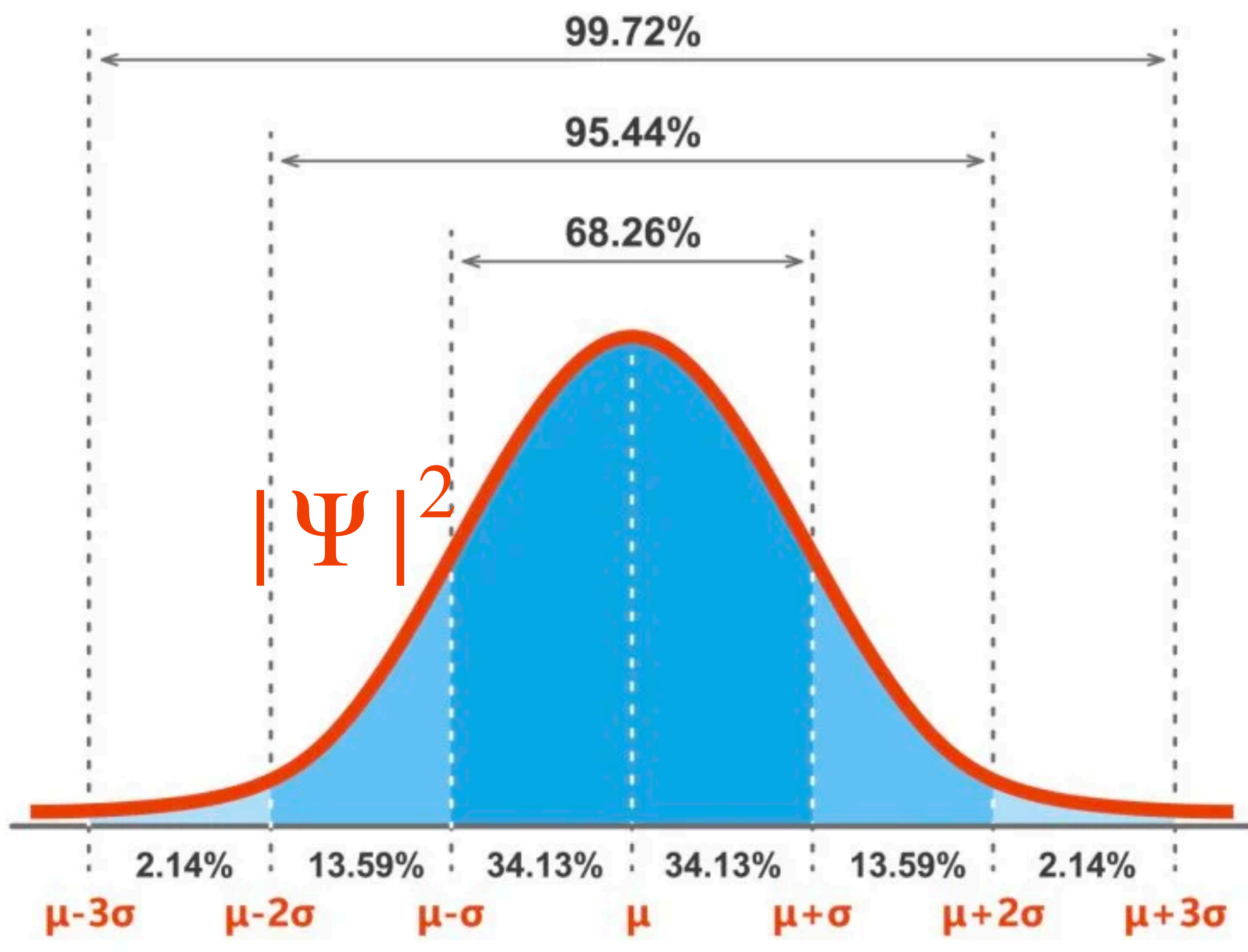

- **Note the use of imaginary numbers! $|\Psi|^2$ is the amplitude of a complex number: $|a+ib|^2 = \sqrt{a^2+b^2}$. Imaginary numbers "are not real" but they are critical to our most accurate theories of reality!!**

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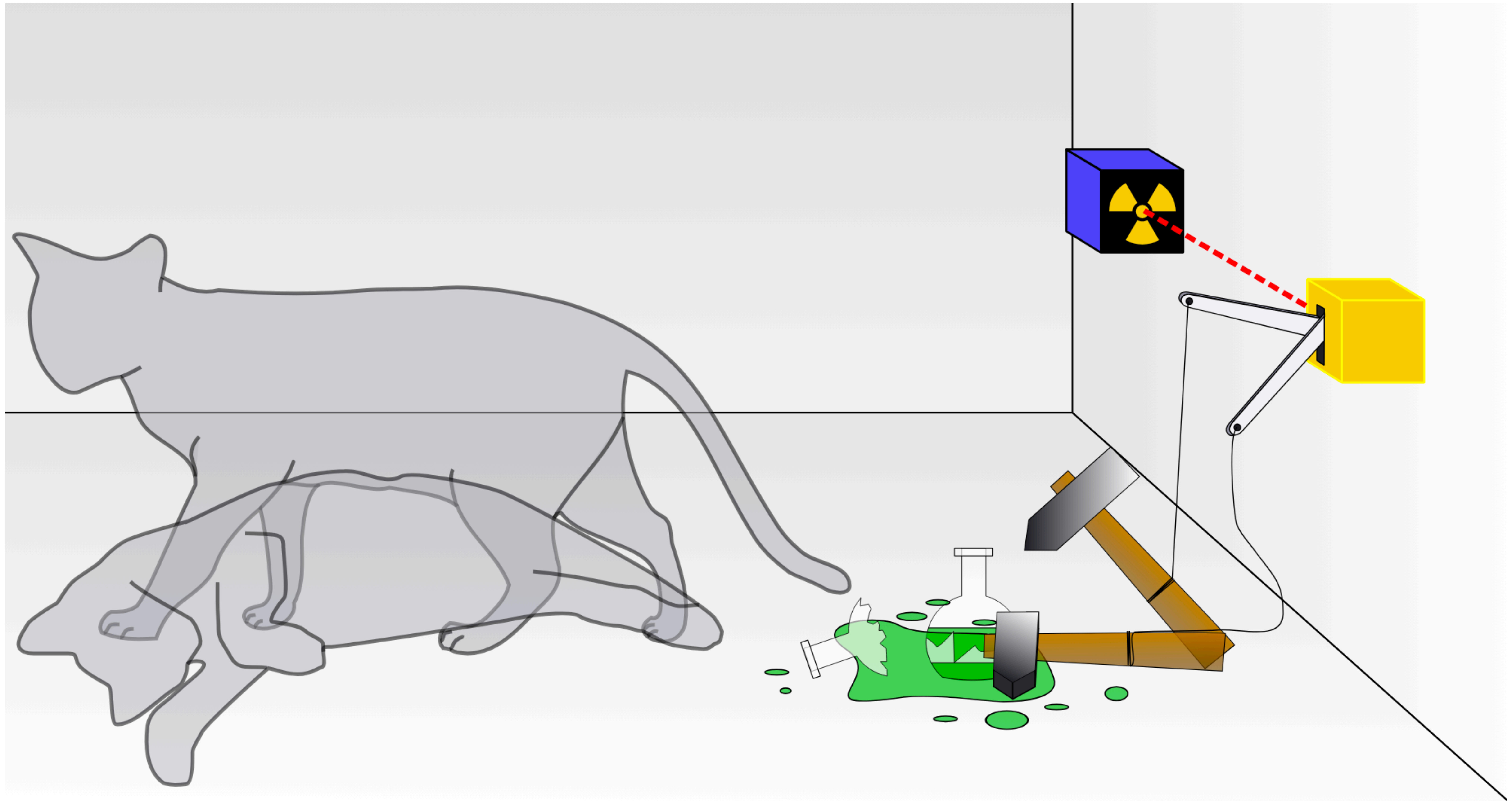
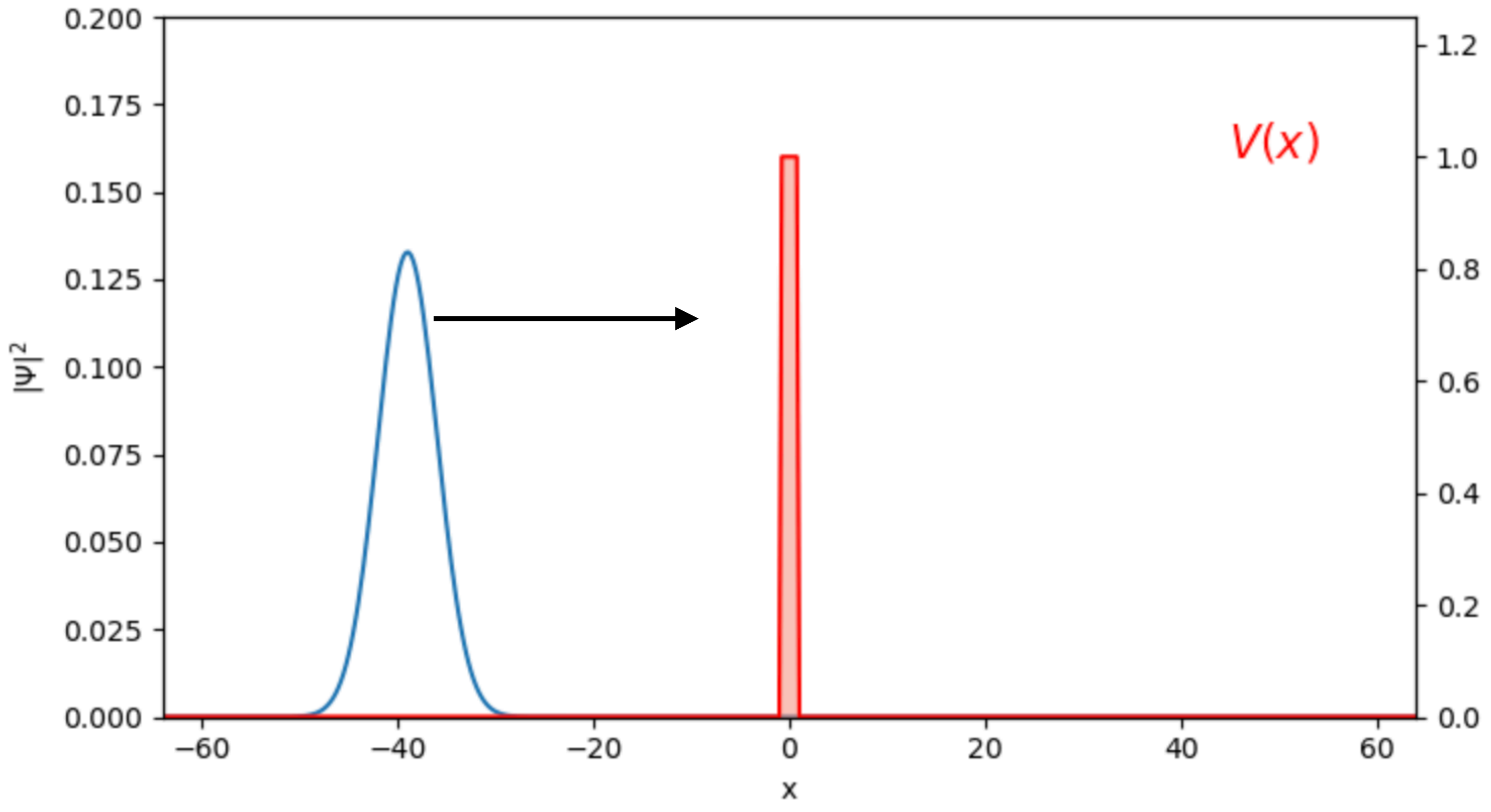
Schrödinger's cat

- 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



$t = 0$

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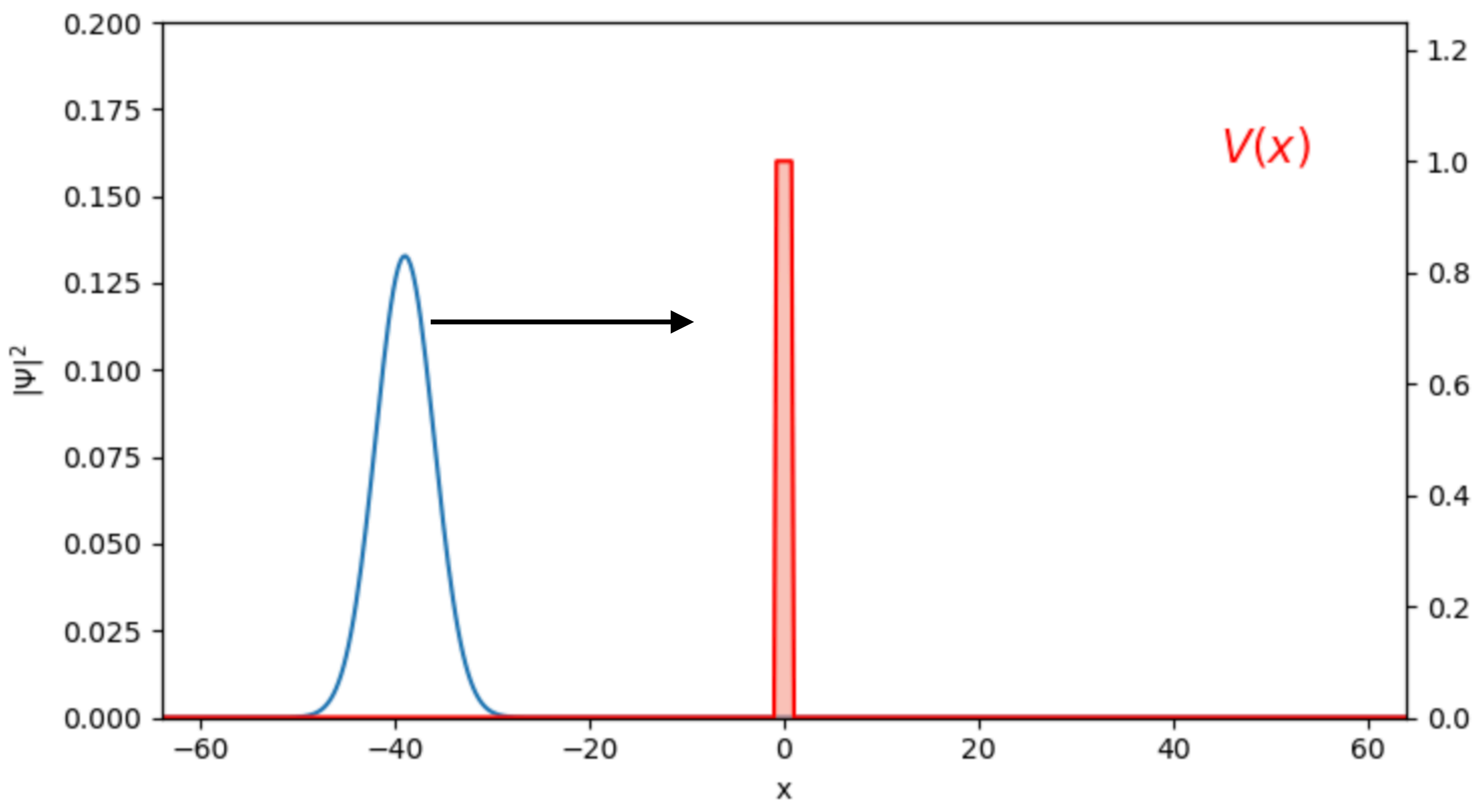
Quantum Tunneling

- **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?



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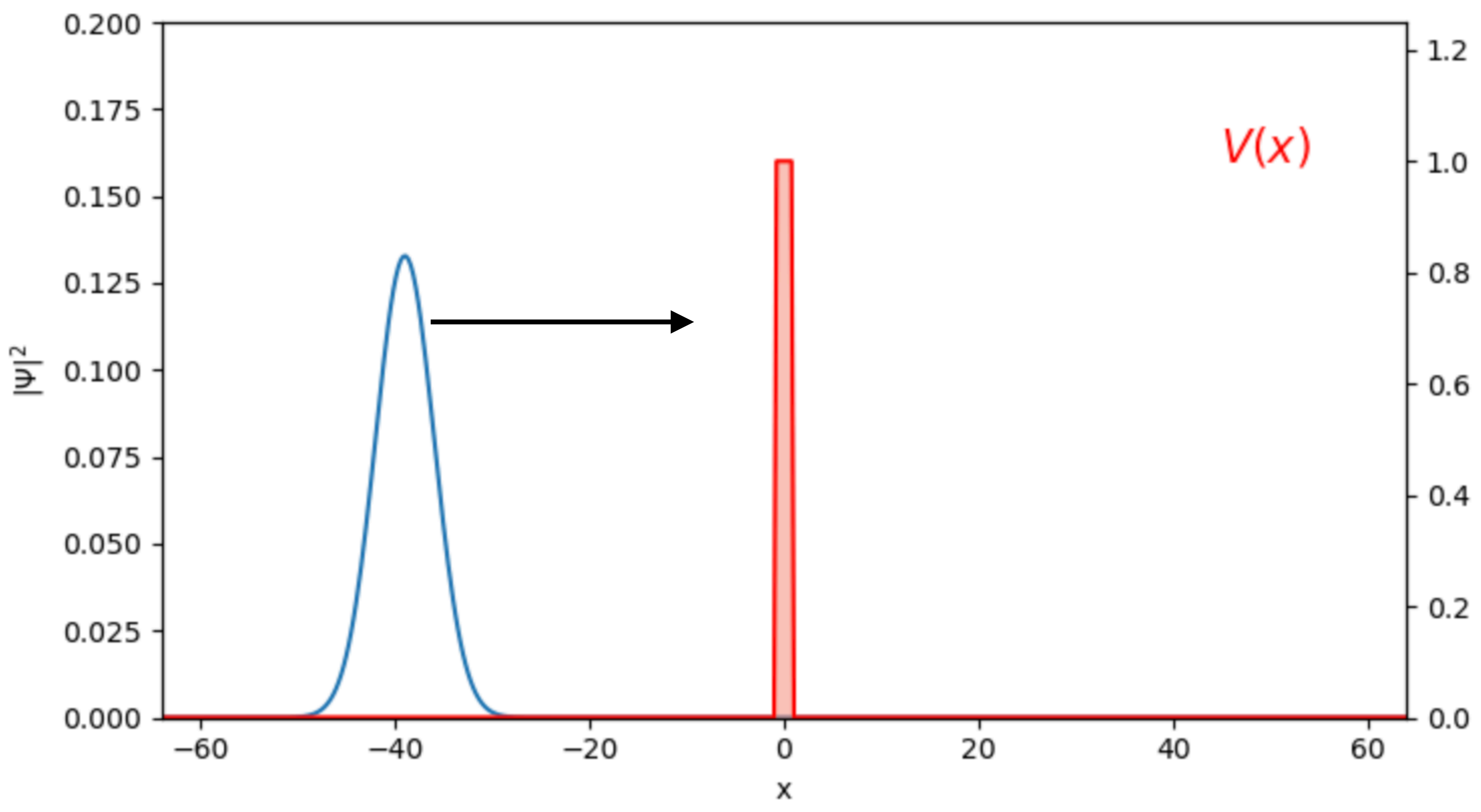

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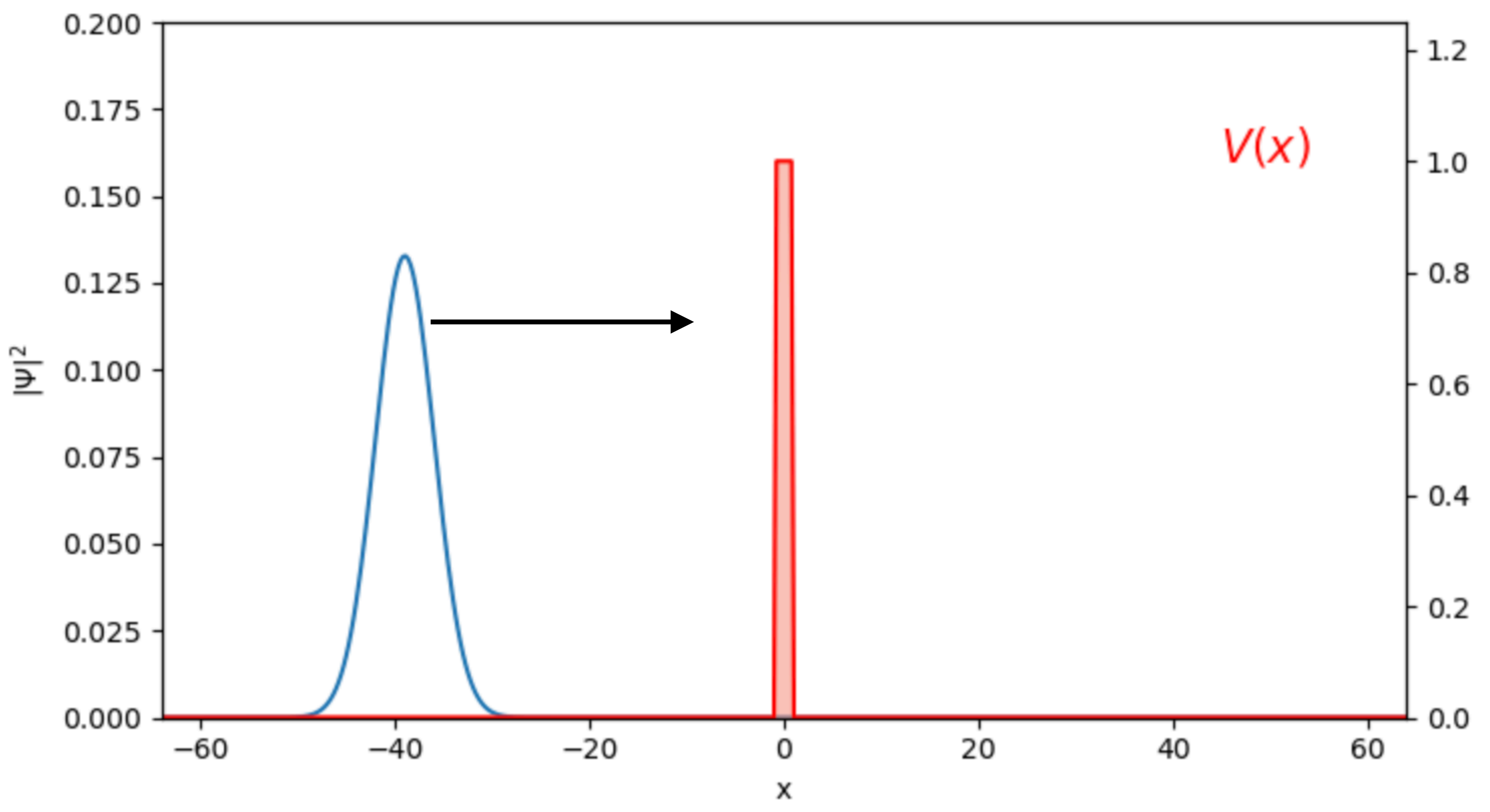

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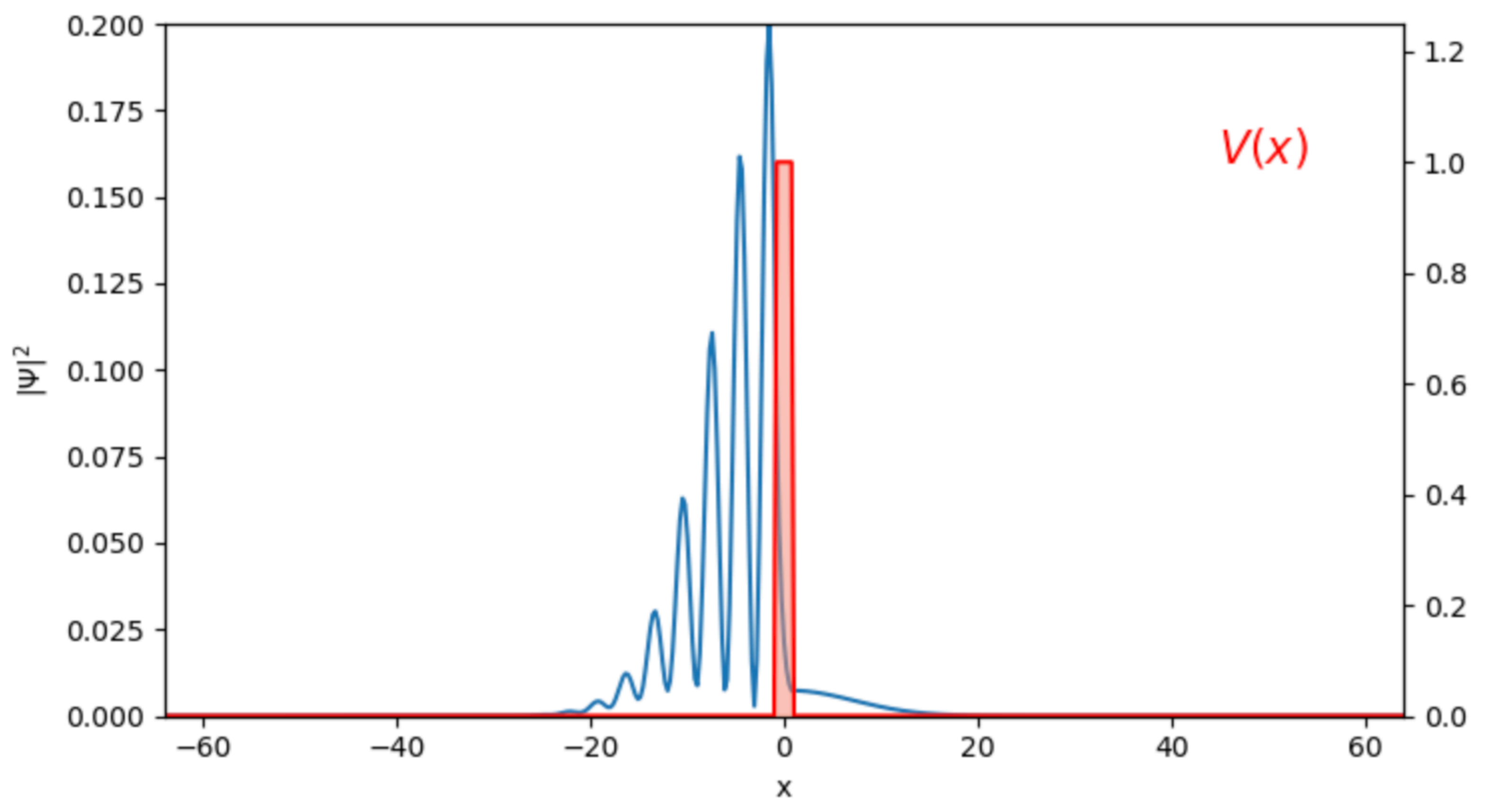
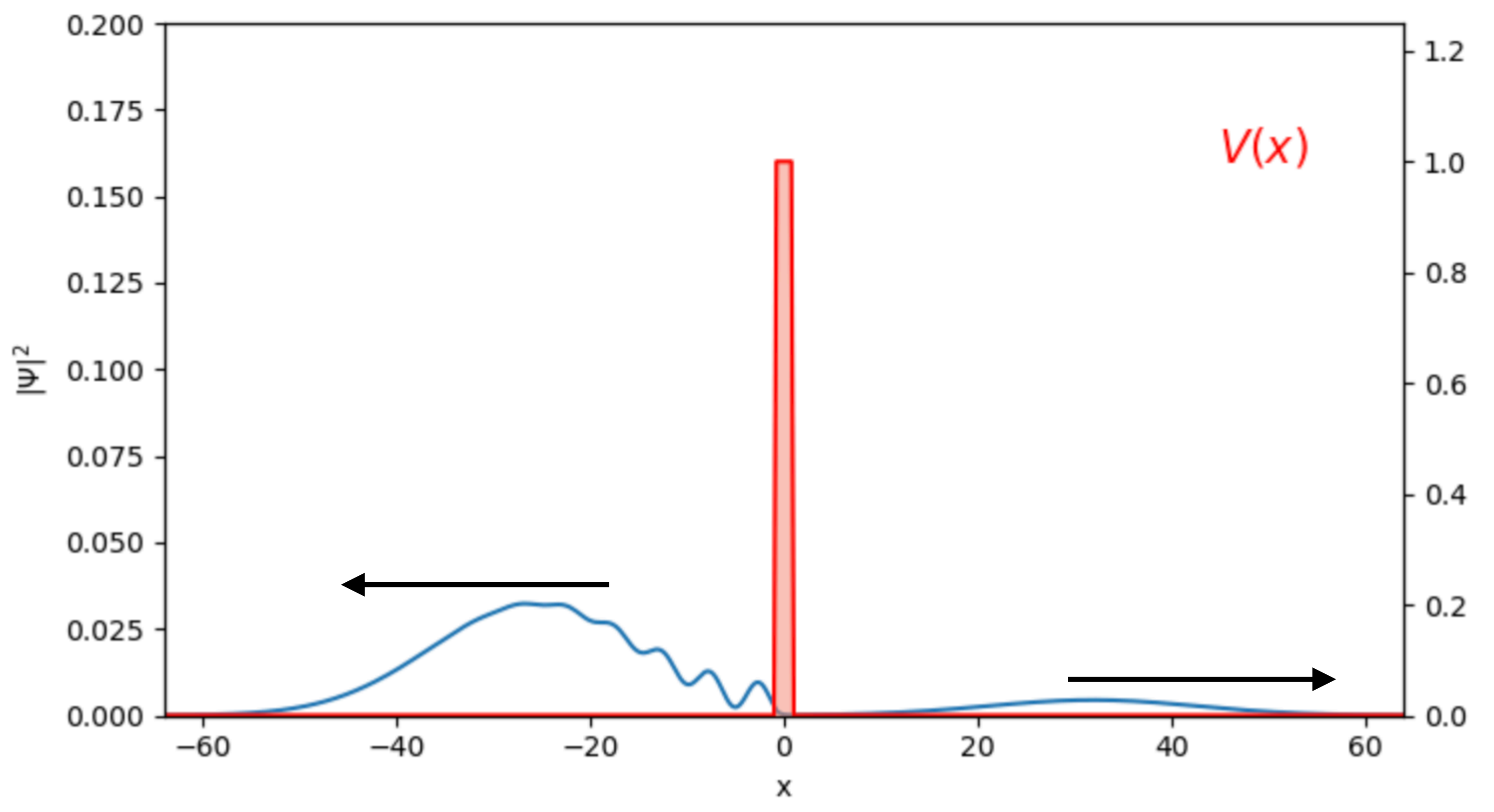


$t = 1$



$t = 2$

Quantum Tunneling

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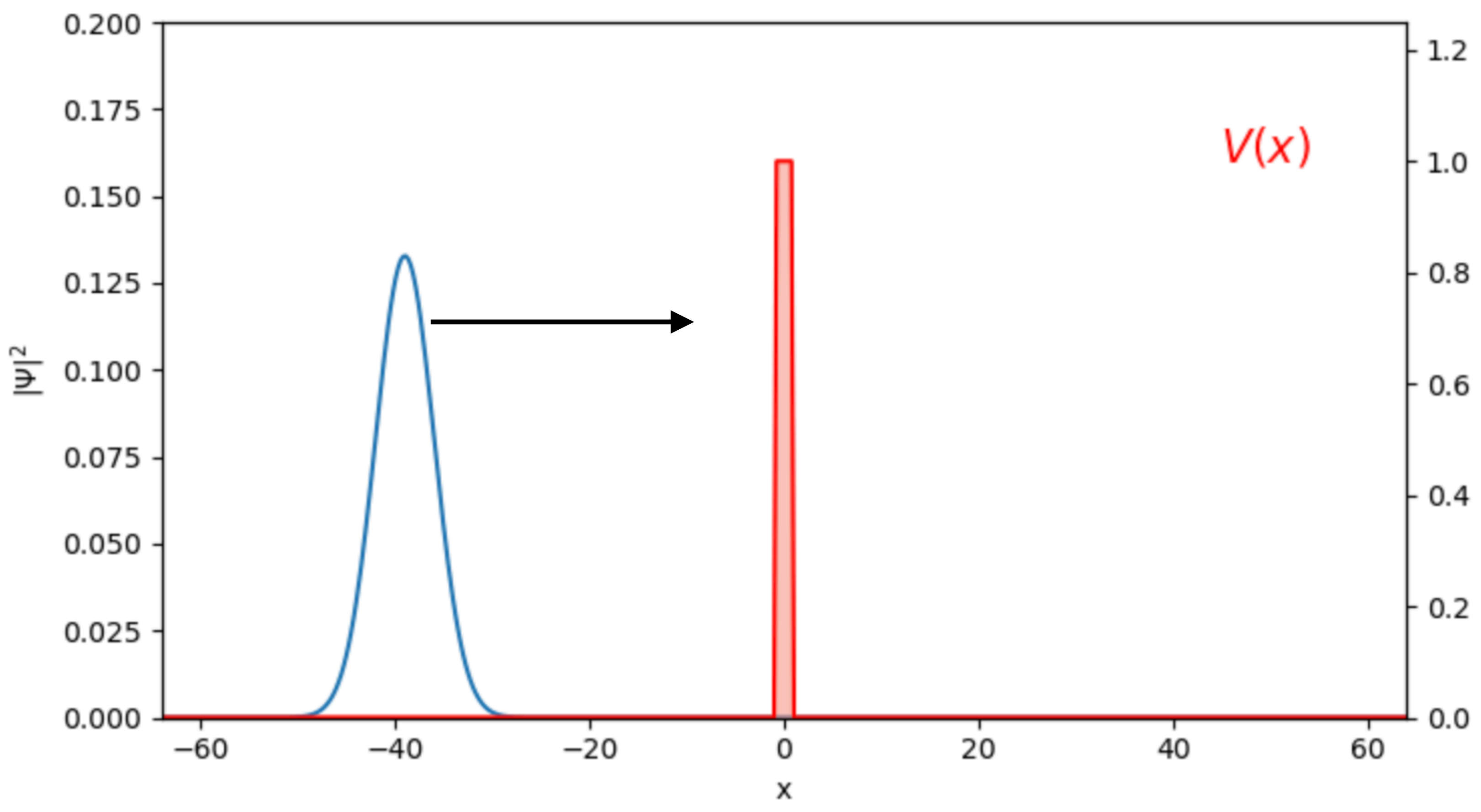
  - What happens?

- **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”**



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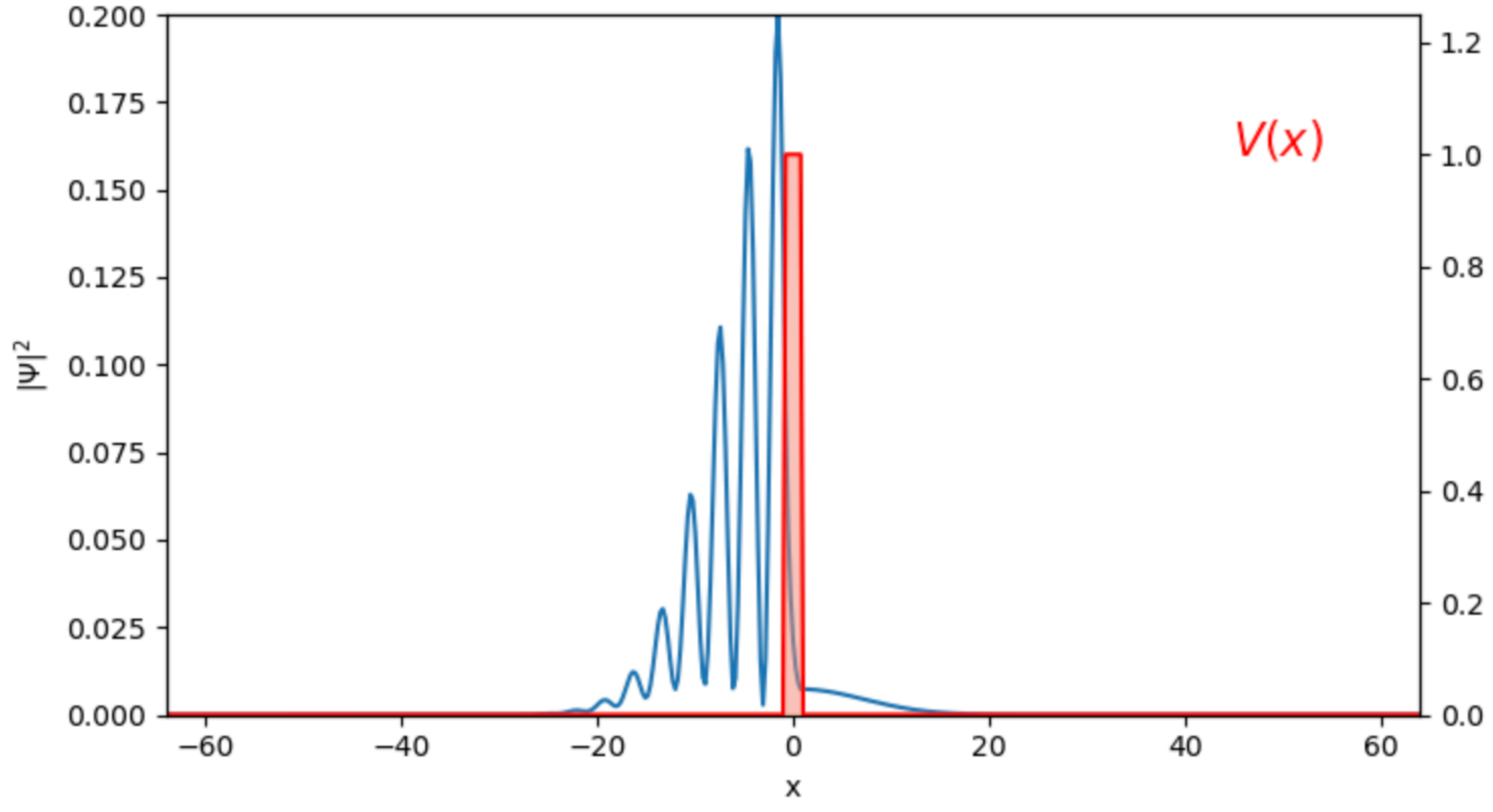

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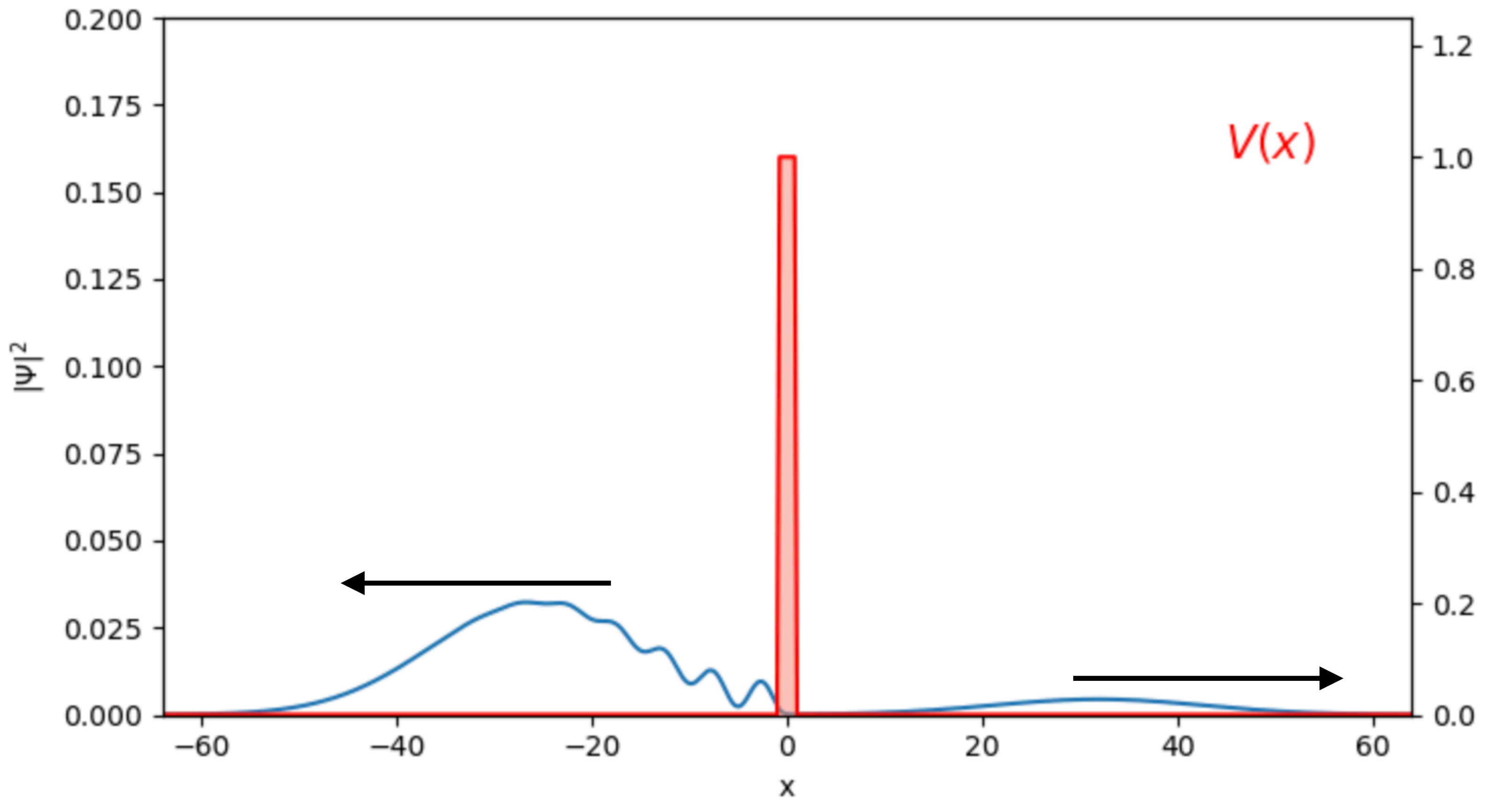

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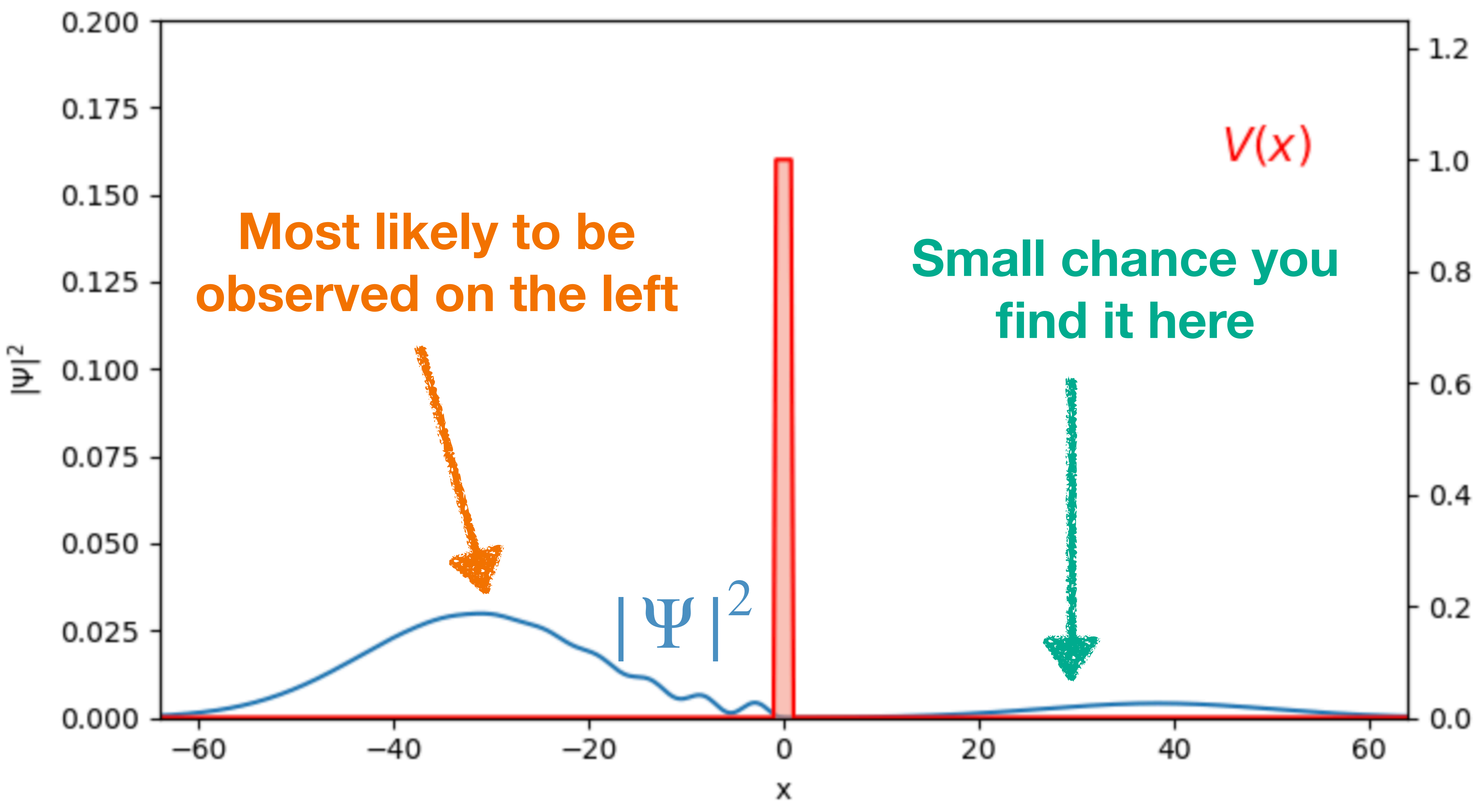
What if we open the box?



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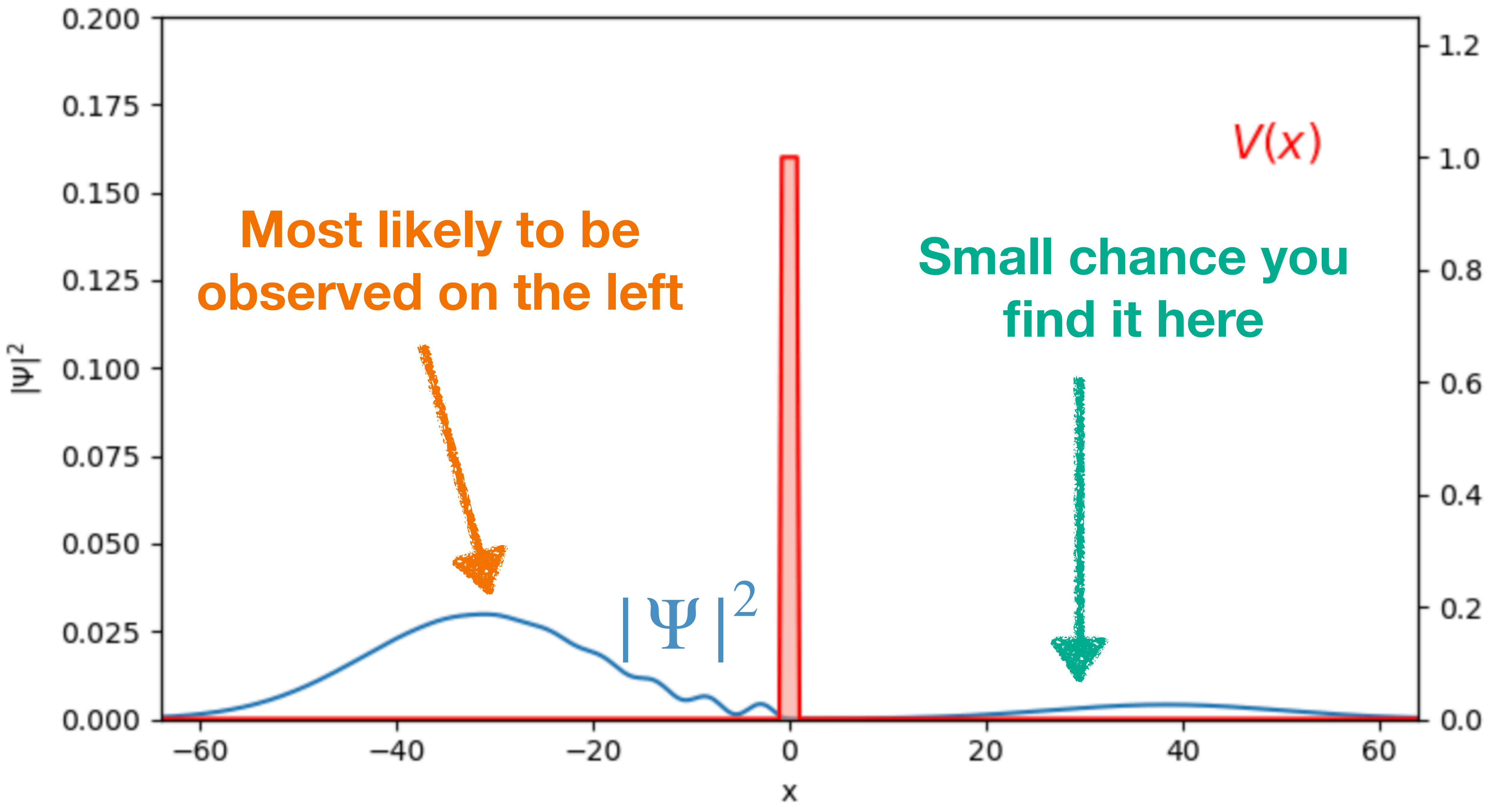
- **We are not simulating wave function collapse, but simply the evolution of the quantum wave function.**



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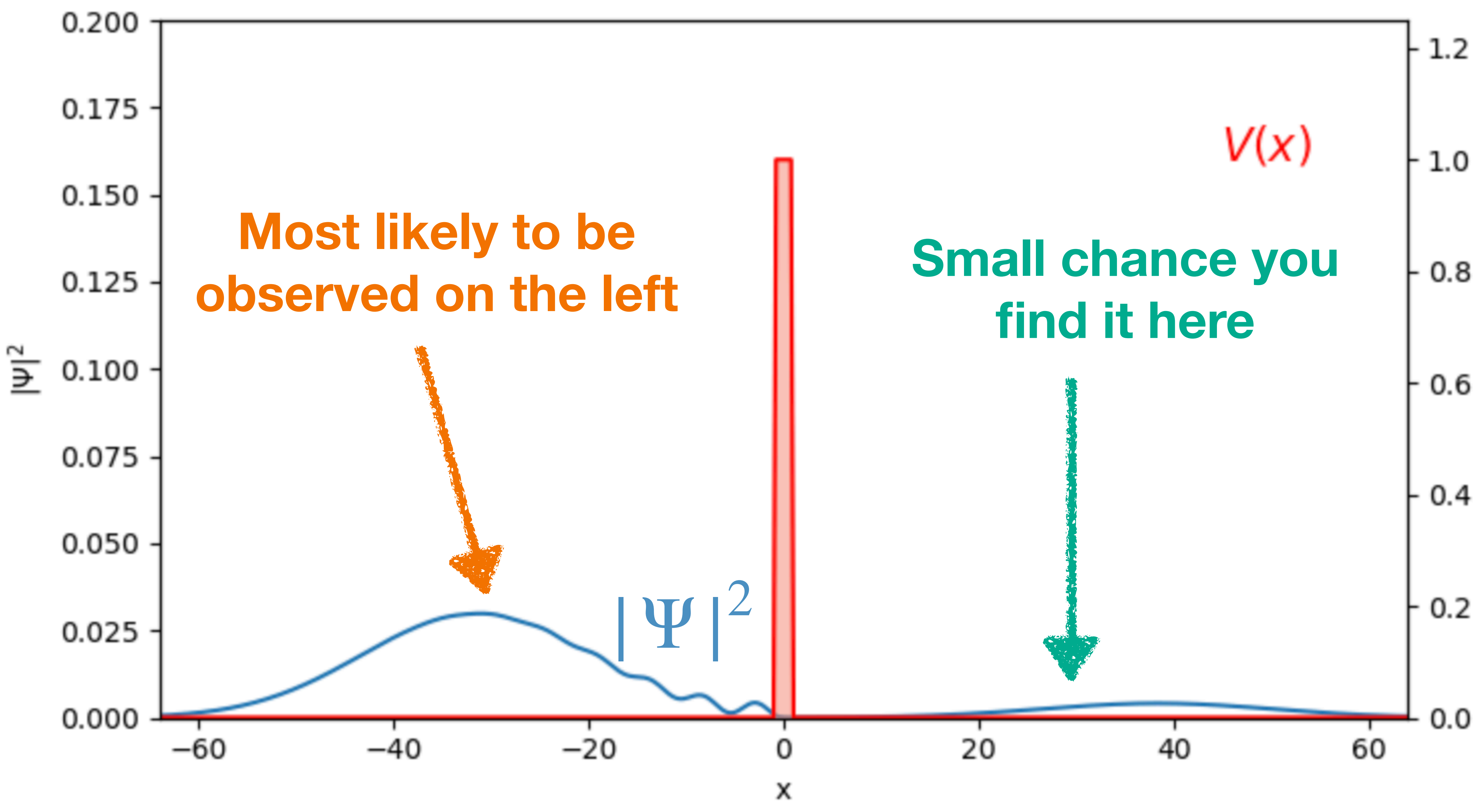
- We are not simulating wave function collapse, but simply the evolution of the quantum wave function.
- If you pause your simulation at a given time, the function currently displayed shows the probability of the particle to be in any particular location (we square the wave function before plotting it)



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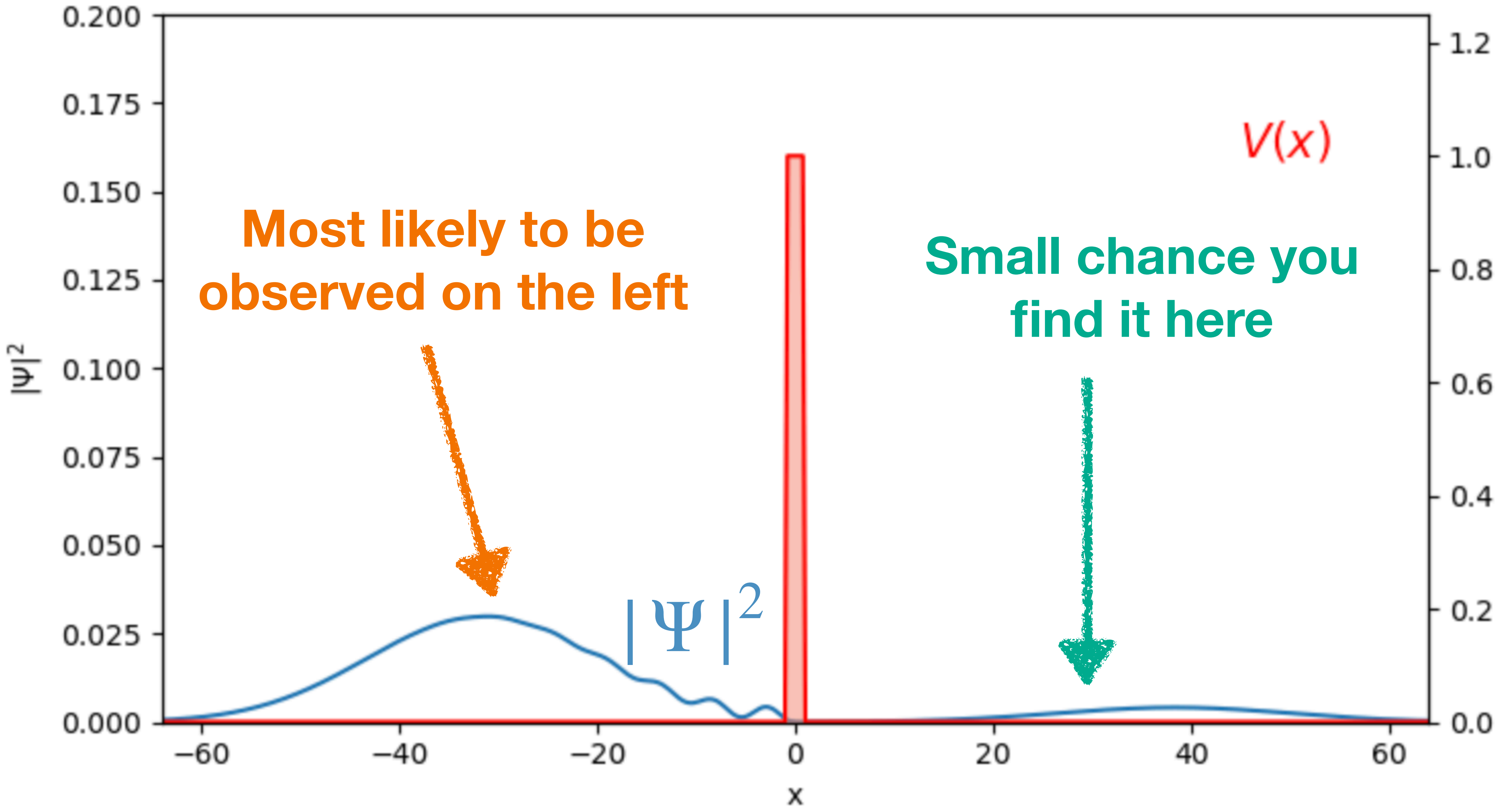
- When you "open the box" you just get the position of the particle. In this case the most likely answer is x=-30, but you could sometimes get x=-20 or -50. If you repeat the experiment rarely, but sometimes, you'll get a positive number.



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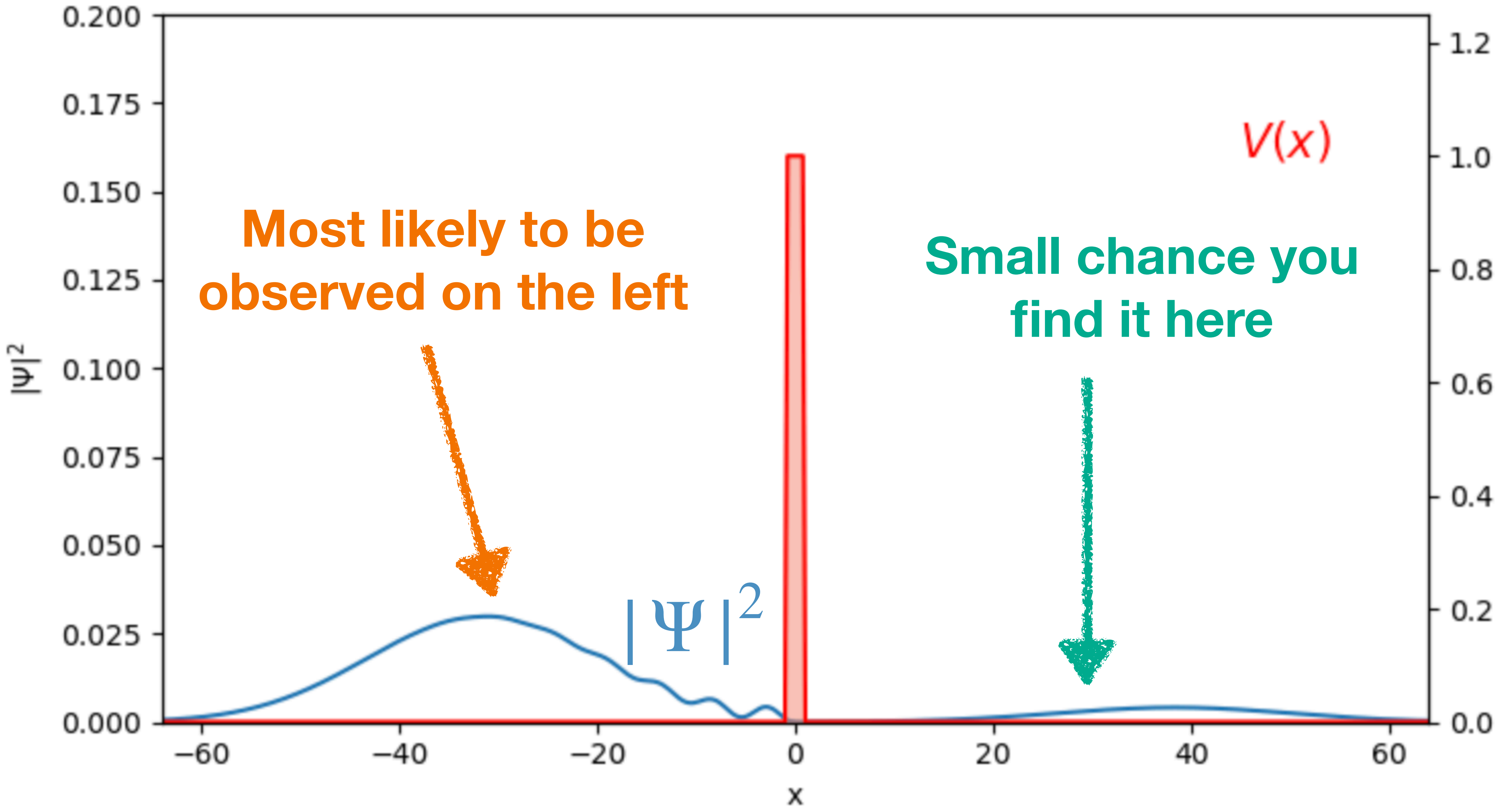
- When you open the box in Schrödinger's thought experiment, you find out if the cat is alive or dead. It will be one or the other, not both.



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- **The Schrödinger Equation is not only a *wave equation* but a *differential equation*. It is an equation with derivatives of functions inside it.**

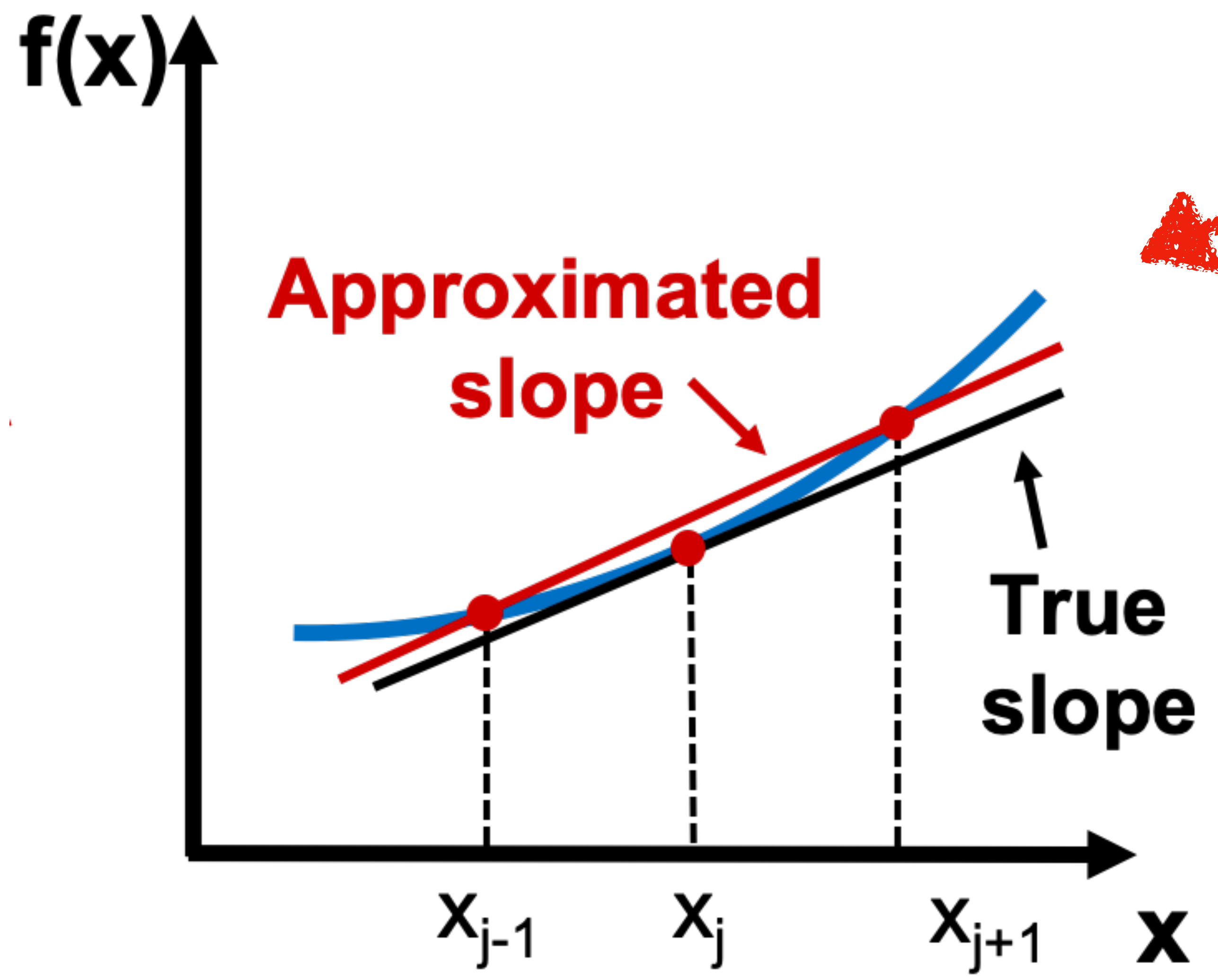
- **Like wave equations, differential equations are *everywhere* in physics:**
  - Newtonian physics: $F = ma = m\frac{d^2x}{dt^2}$
  - Fluid dynamics
  - Schrödinger equation and other quantum wave equations

- **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.**