PARTICLE IN A BOX - Quantum Tunneling

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QUANTUM TUNNELING

Quantum tunneling is a quantum mechanical phenomenon where a wave function that represents the status of some energy particles can propagate through a potential wall.

In classical mechanics, objects obey rigid and intuitive laws of motion; a ball left to roll down a hill will not have enough energy to roll over a second, taller hill.

The same behavior might be expected of charged particles (like electrons) in "hills" made of electric potentials. However, the Schrodinger equation, which governs the dynamics of quantum particles, suggests that particles can cross potentials which have more energy than the particles themselves. This phenomenon is known as quantum tunneling.

In this project, we established the existence of quantum tunneling and investigated its mathematical properties using tools from real analysis and partial differential equations.

INFINITE SQUARE WELL

We studied three variations of the infinite square well problem. The model describes a 1D quantum system of a particle trapped within an "infinite square well". This means the particle's movement is restricted to a predefined interval of the real number line. Mathematically, the well is a function that maps position to a potential energy:

$$V(x) = \begin{cases} 0 & x \in (-1,1) \\ \infty & \text{else} \end{cases}$$

Since the particle's total energy is the sum of its kinetic and potential energy, when the potential energy is infinite, the particle's kinetic energy is zero. This restriction is represented in each image by the gray region region.

- **Free Particle**
- **Uniform Potential Wall**
- **Arbitrary Potential Wall**

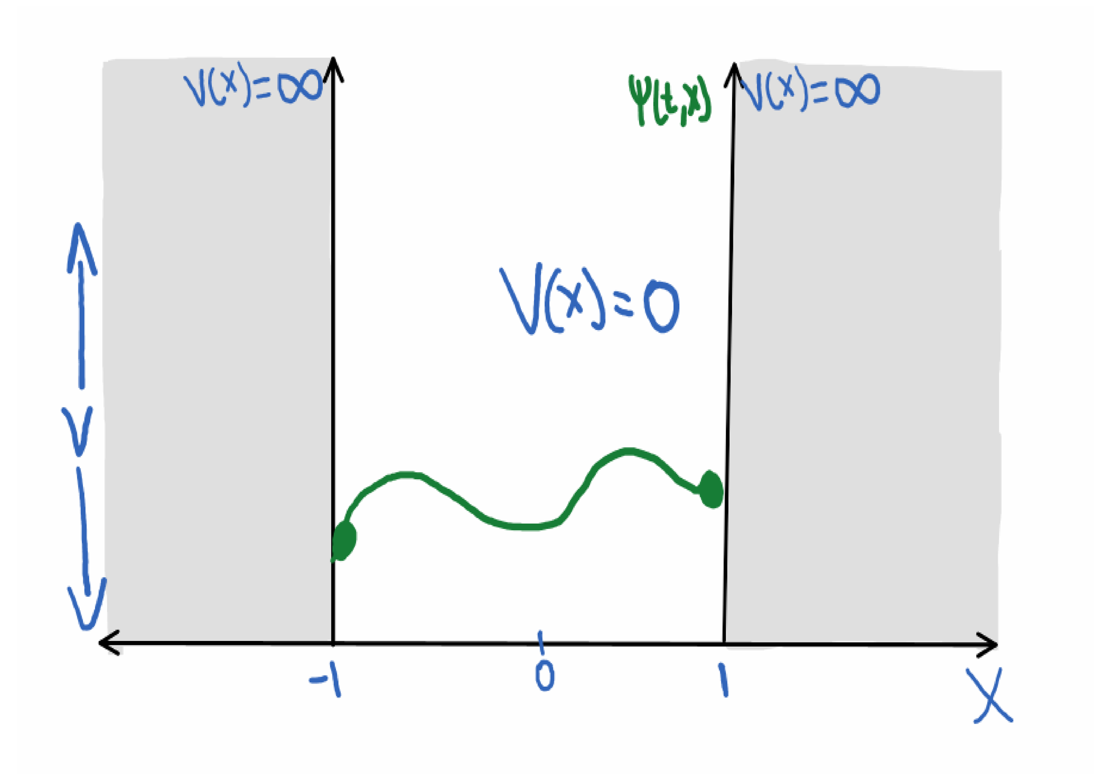
OUR MAIN THEOREM

Let $\psi(t,x)$ and $\phi(t,x)$ be wavefunctions of a free particle system and barrier-present system, respectively. If 2ε denotes the width of a potential barrier, then for some point in time $T > 0$, quantum tunneling occurs when:

$$\lim_{\varepsilon \to 0} \left(\sup_{t \in [0,T]} ||\psi(t,x) - \phi(t,x)||_{L^2} \right) = 0$$

FREE PARTICLE SYSTEM

- This is the most simple case.
- $\psi(t,x)$ is the wave function of a quantum particle that is free to move between $x = -1$ and $x = 1$.
- Comparing $\psi(t,x)$ to more detailed models provided the basis of our investigation into quantum tunnelling.



GOVERNING EQUATIONS

$$i\partial_t \psi(t,x) = -\partial_x^2 \psi(t,x)$$
$$t \in [0,\infty), \quad x \in (-1,1)$$
$$\psi(0,x) = \psi_0(0)$$
$$||\psi_0||_{L^2} = 1$$

- i = imaginary unit
- t = time variable
- x = spatial variable

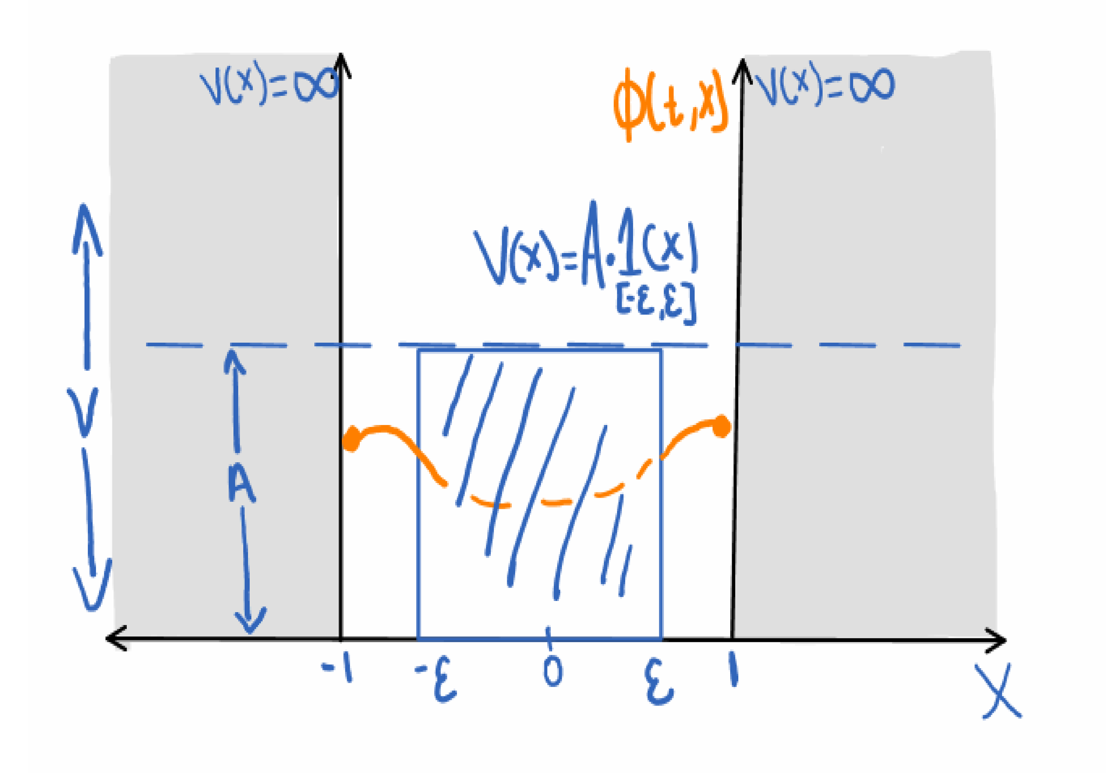
ENERGY OPERATOR

- This operator allowed us to re-express our PDE systems as integral equations.
- For some wave function φ modelling a particle-in-a-box, we obtained the transformed function:

$$\tilde{\phi}(t,x) := e^{-it\partial_x^2} \phi(t,x)$$

UNIFORM POTENTIAL BARRIER

- $\phi(t,x)$ is the wave function of a particle whose path is obstructed by a rectangular barrier.
- Proved existence of tunnelling by comparing behavior of $\phi(t,x)$ and $\psi(t,x)$.



UNIFORM POTENTIAL GOVERNING EQS

$$i\partial_t \phi(t,x) = -\partial_x^2 \phi(t,x) + A \cdot 1_{[-\varepsilon,\varepsilon]}(x)\, \phi(t,x)$$
$$t \in [0,\infty), \quad x \in (-1,1)$$
$$\phi(0,x) = \psi_0(0)$$

- i = imaginary unit
- t = time variable
- x = spatial variable

OPERATOR PROPERTIES

To help prove our result, we investigated operator $e^{-it\partial_x^2}$

(1) $e^{-is\partial_x^2} \cdot e^{-it\partial_x^2} = e^{-i(s+t)\partial_x^2}; \quad \forall s,t \in \mathbb{R}$

(2) $e^{-it\partial_x^2}\Big|_{t=0}$

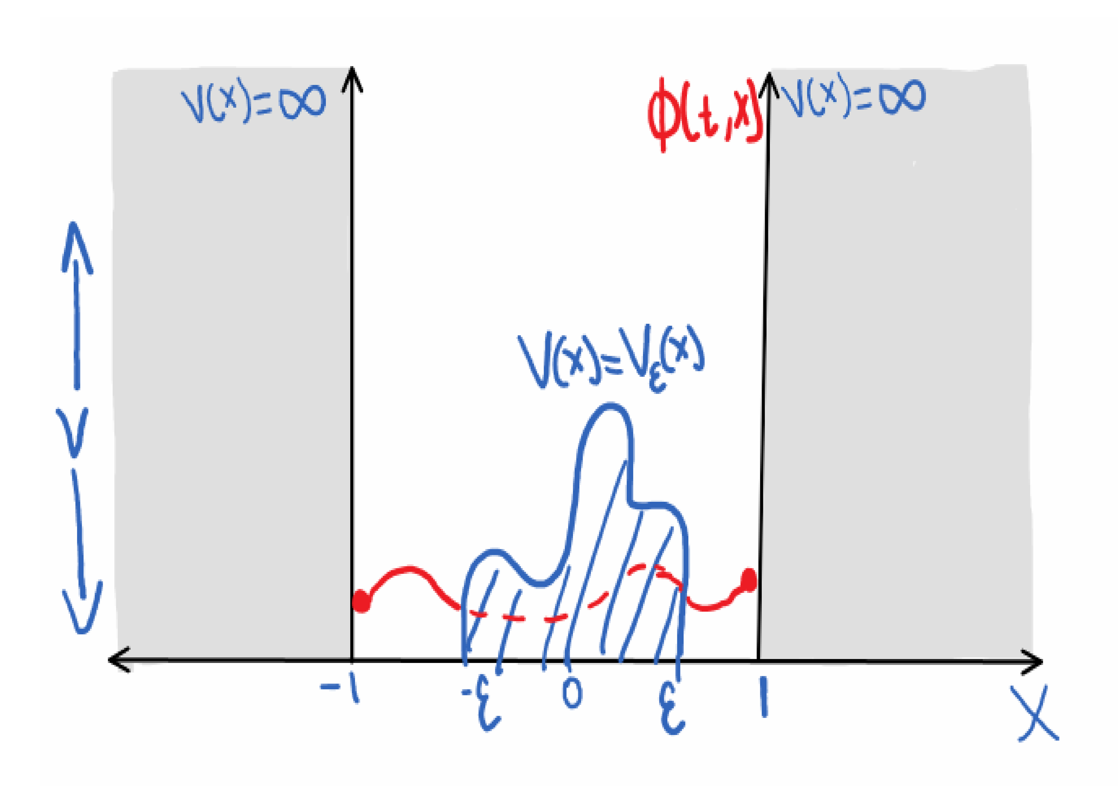
(3) $||e^{-it\partial_x^2} \cdot f||_{L^2} = ||f||_{L^2}$

(4) $\partial_t \left(e^{-it\partial_x^2} \cdot f(t,x) \right) = -i\partial_x^2 e^{-it\partial_x^2}$

(5) $\partial_x^2 e^{-it\partial_x^2} = e^{-it\partial_x^2} \partial_x^2$

ARBITRARY POTENTIAL BARRIER

- $\phi(t,x)$ is the wave function of a particle whose path is obstructed by an arbitrarily shaped potential barrier $V_\varepsilon(x)$.
- Confirmed that tunneling still occurs.
- Analyzed the properties of $V_\varepsilon(x)$ to develop a set of necessary conditions for tunnelling to occur.



ARBITRARY POTENTIAL GOVERNING EQS

$$i\partial_t \phi(t,x) = -\partial_x^2 \phi(t,x) + V_\varepsilon(x)\, \phi(t,x)$$
$$t \in (0,\infty), \quad x \in (-1,1)$$
$$\phi(0,x) = \psi_0(0)$$

- i = imaginary unit
- t = time variable
- x = spatial variable

TUNNELLING PROPERTIES OF V_ε

1. $V_\varepsilon(x) \in L^2 \cap L^\infty$
2. $\sup ||V_\varepsilon(x)||_{L^\infty} < \infty$
3. $\lim_{\varepsilon \to 0} ||V_\varepsilon||_{L^2} = 0$

REFERENCES

T, Arbogast and J, Bona. Methods of Applied Mathematics. (corrected version) ed., Department of Mathematics, and Institute for Computational Engineering and Science , 2007.

W, Rudin Principles of Mathematical Analysis. Third ed., McGraw-Hill Inc., 1964.