Course Structure

- 1 - Waves as particles - the Photon [3 hours]
- 2 - Atomic theory from 400 BC to 1913 [2 hours]
- 3 - Particles as Waves [1 hour]
- 4 - Elements of Quantum Mechanics I - The wave-function [3 hours]
- 5 - Elements of Quantum Mechanics II - Energy in quantum mechanics [6 hours]

Wavefunctions - Summary of properties

- A **wavefunction** is a function of position which:
  - is a **positive** and / or **negative** (and/or complex) number for all values of x (can be zero).
  - ψ(x) is **normalised**.
  - ψ(x) is **continuous**.
  - Probability of position measurement via the **Born rule**:

$$\mathrm{Prob}(a \leq x \leq b) = \int_a^b |\psi(x)|^2 dx$$

Normalisation

- Sometimes we calculate wave-functions, but they are **not normalised** (a common result of standard calculation techniques).
- Fortunately, for most functions, we can **convert** them into **normalised wavefunctions** by a **simple method**:
- Consider function $\psi_1(x)$ which satisfies:

$$\int_{-\infty}^{\infty} |\psi_1(x)|^2 dx = N \neq 1$$

- If we divide $\psi_1(x)$ with $\sqrt{N}$ we achieve a **normalised** function
- $\psi_2(x)$ is **normalised**.

$$\psi_2(x) = \frac{\psi_1(x)}{\sqrt{N}} \qquad \int_{-\infty}^{\infty} |\psi_2(x)|^2 dx = \frac{N}{N} = 1$$

Expectation values

- The expectation value represents this expected mean value after a very large number of repetitions.
- From:

$$\langle x \rangle = \int_{-\infty}^{\infty} \rho(x) x \; dx$$

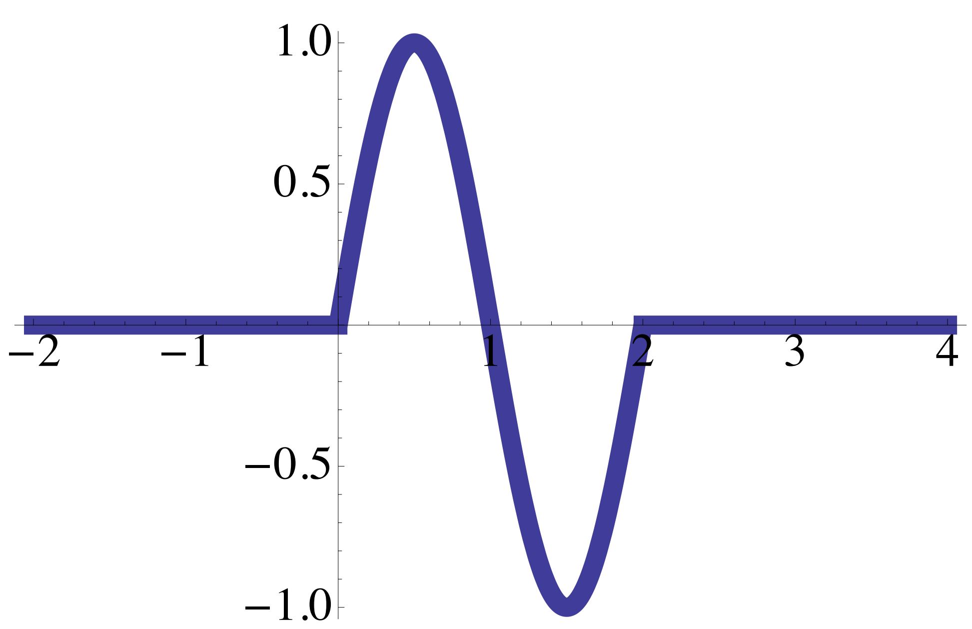
- We obtain:

$$\langle x \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 x \; dx$$

Why the wave function?

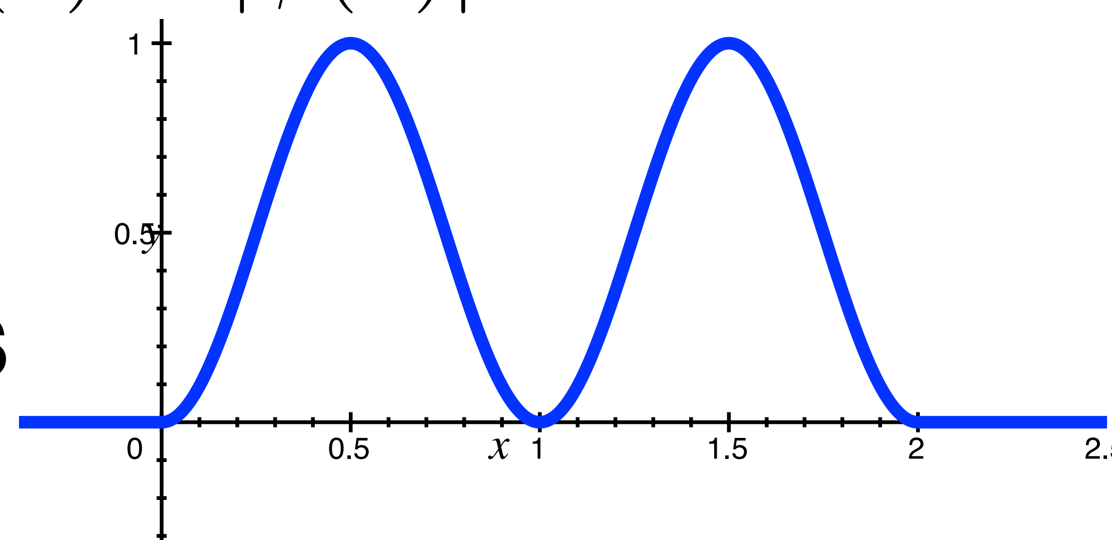
- So far, we have done nothing with the wave function other than **calculate probabilities**.
- So why use wave functions at all?
- Why not just work with **probabilities**?
  - We need **negative values** to achieve **destructive interference**!

$\psi(x)$



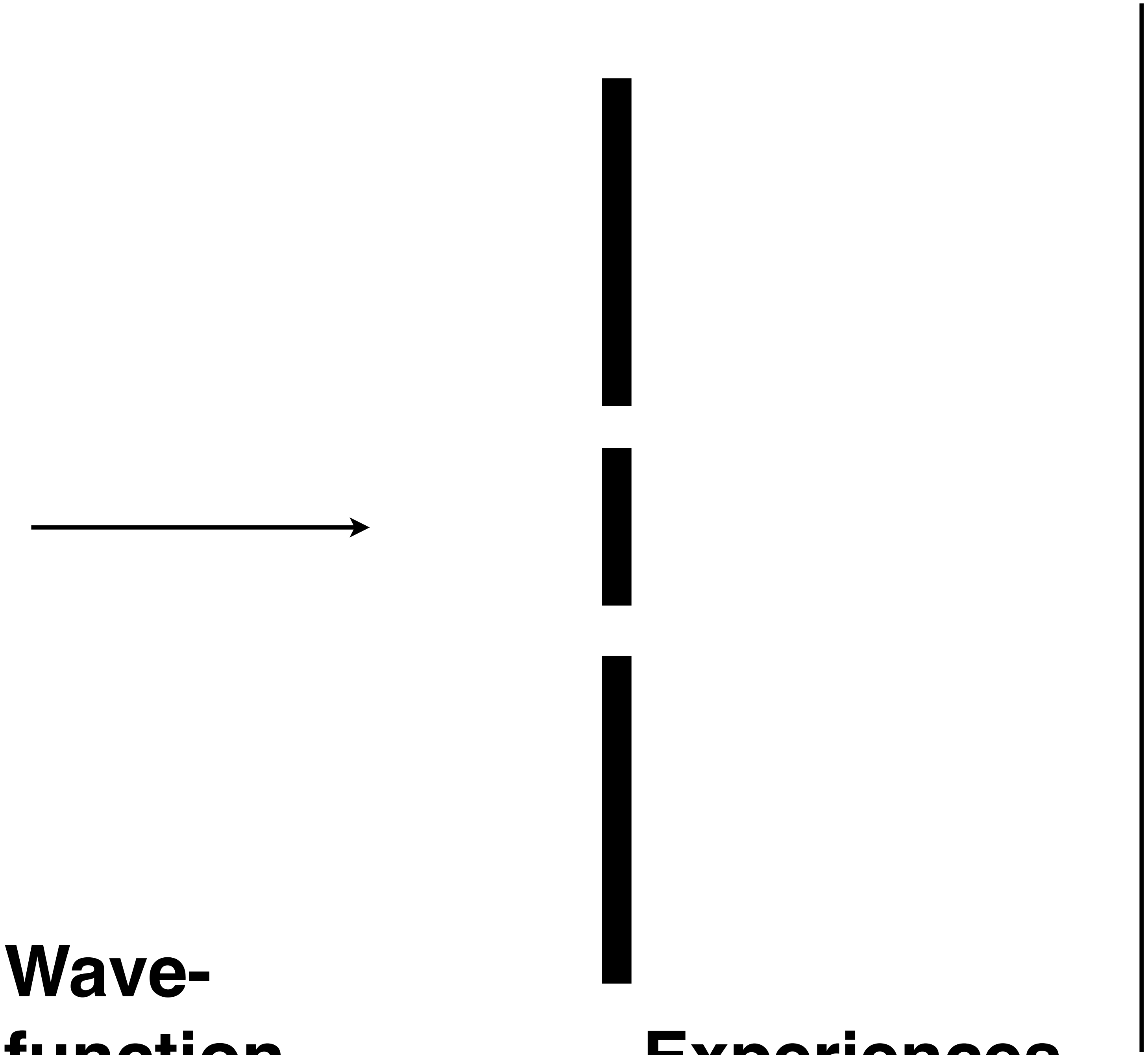
vs

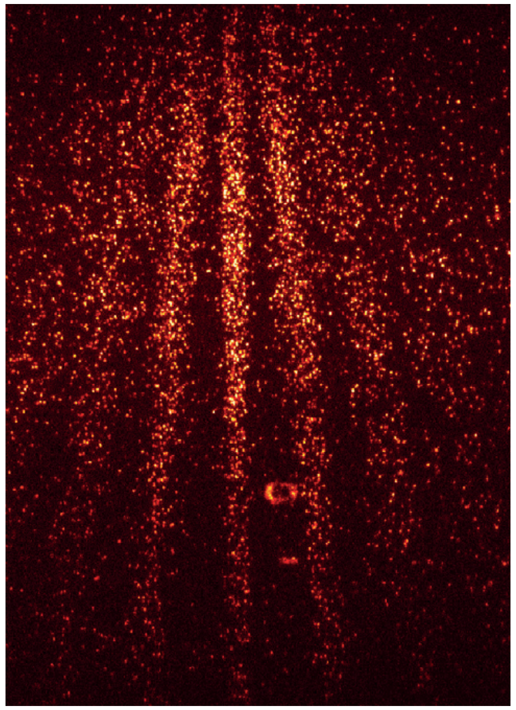
$$\rho(x) = |\psi(x)|^2$$



Double-slit experiment

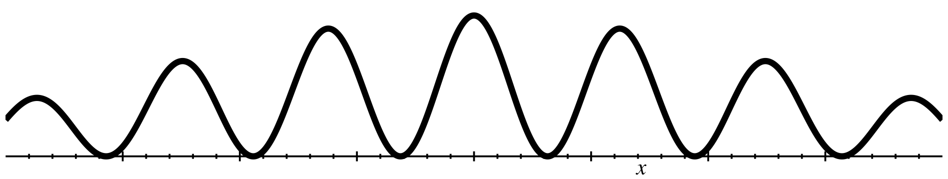
– **Jönsson** (1961): **Electrons**





Probability density:

$$\rho(x) = |\psi(x)|^2$$



Wave-function evolves ”as a wave”

Experiences wave interference

Clicks on screen follow Born rule.

Evolution in time

Erwin Schrödinger

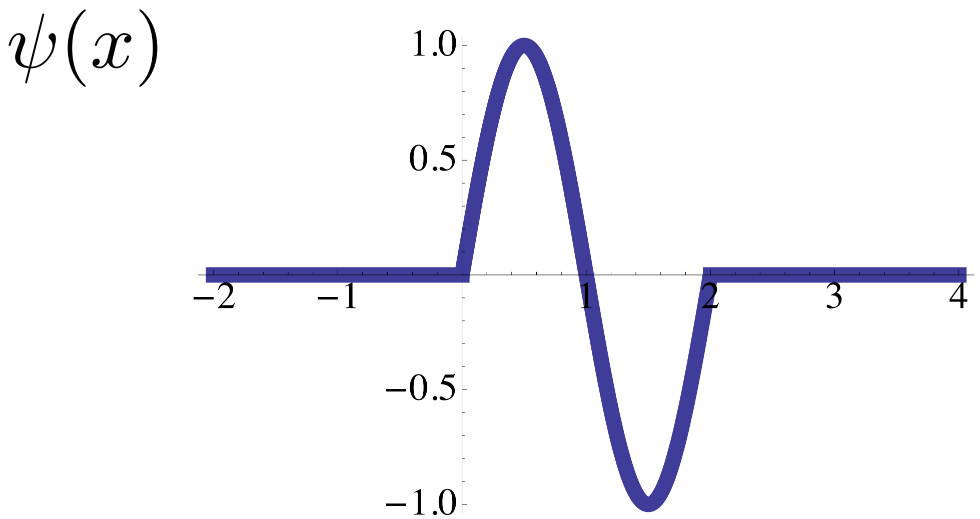
- When not being measured, wave-functions evolve in time according to the **Time Dependent Schrödinger Equation**.

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

- We will **not** study this in this course! (2nd year)
- It is **similar** to the equation followed by **classical waves** (e.g water), but with some important differences.
  - E.g. It contains the **complex number i** (i = √(-1))
- For the purposes of this course, it suffices to think of the wave function "**evolving like a wave**".

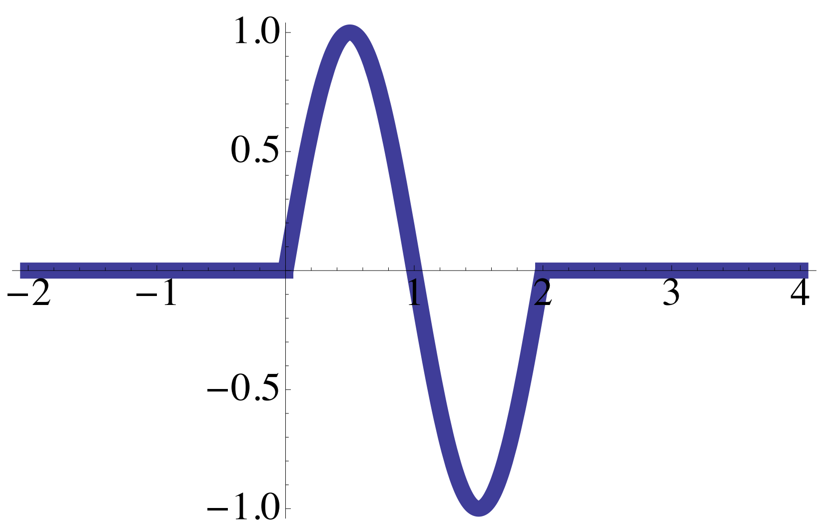
Importance of ψ(x)

- Quantum particles **do not** have a “position” in a classical sense.
- Instead, they have a **wave-function**, from which probabilities of position can be computed from the Born rule.
- In quantum mechanics, we don’t ask
  - what is the position of a particle?
  - what is its orbit (e.g. Bohr model)?
- To **characterise** a particles position and motion, we must determine its **wave-function**.

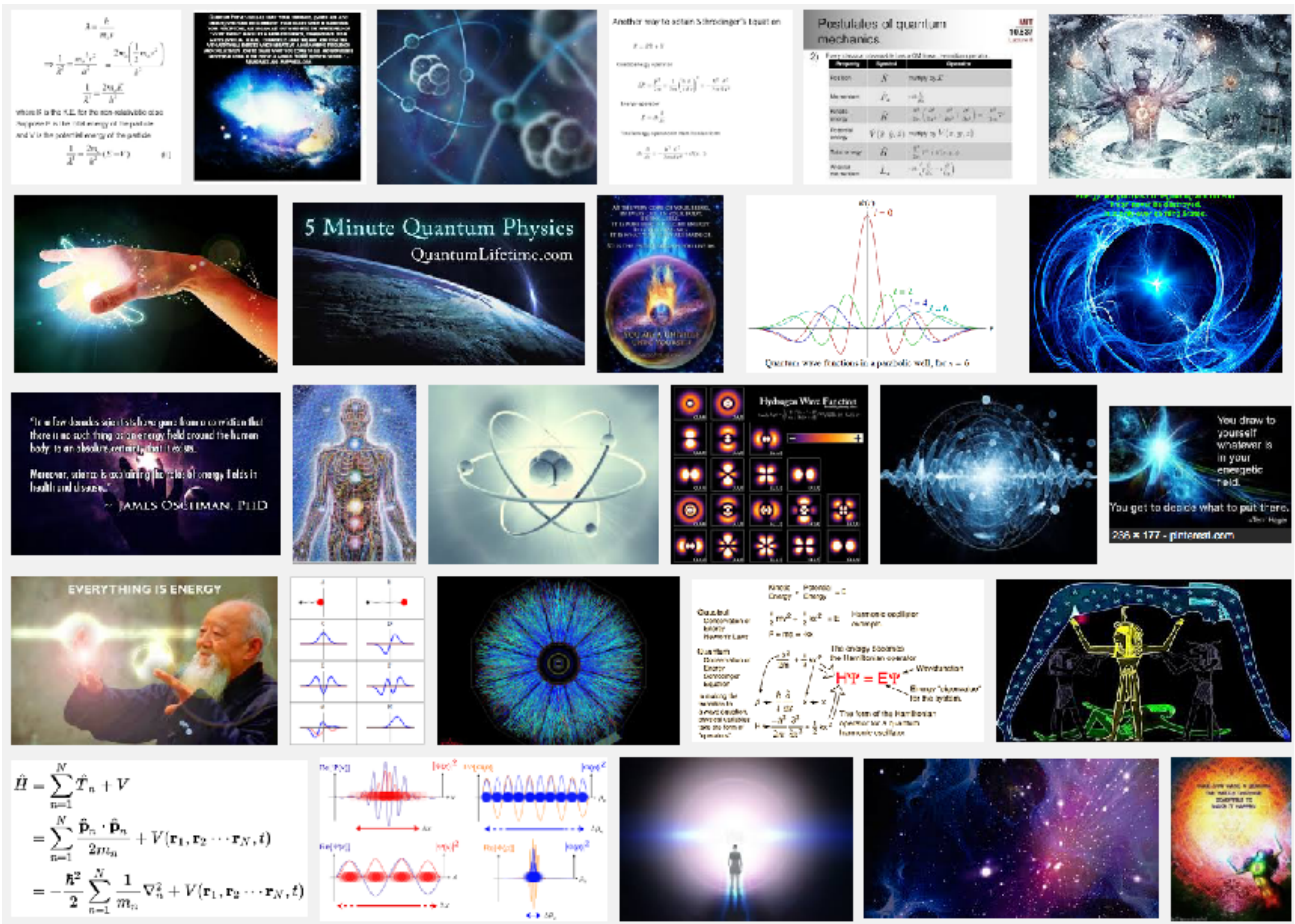


Summary of Part 4

- We revised **probability** for discrete variables and introduced **probability density** for **continuous variables**.
- We introduced the wave-function, studied its properties, and the **Born rule** for calculating **probabilities**.
- We saw how the combination of **wave evolution** with **Born rule** probabilities explains the double-slit experiment with particles.
- We explored **de Broglie** waves, and saw that the **Heisenberg uncertainty principle** forbids particles from having a perfectly defined momentum.



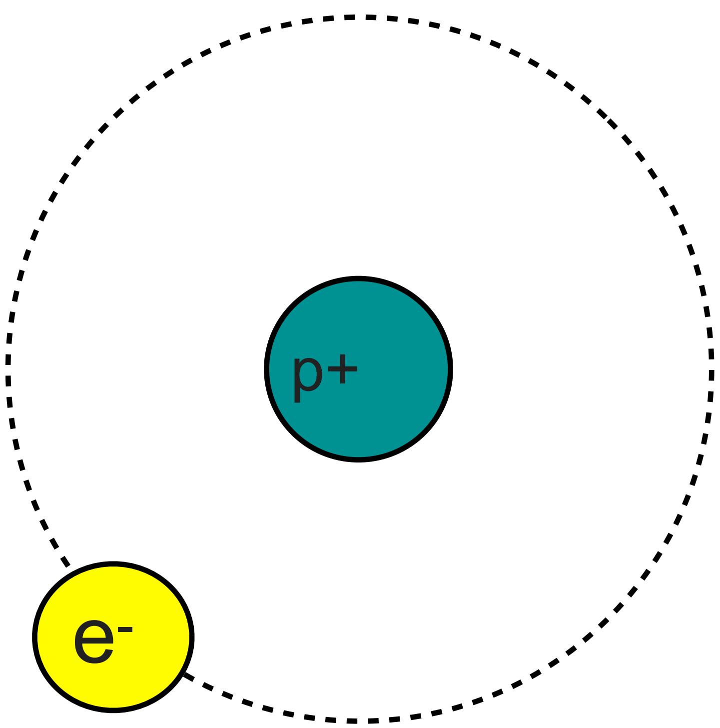
Part 5a: Energy in Quantum Mechanics



Google Image Search: “Energy in Quantum Mechanics”

Towards a quantum atomic model

- We wish to construct a **quantum model** of the **atom**.
- This means, for example, in a **Hydrogen atom**, we wish to identify the allowed **wave-functions** of the **electron**.
- The **wave-function** of the electron which will replace the **orbit** of the **Bohr model**.
- To calculate this - we need to study **Energy in Quantum Mechanics**.
- The theme of **Part 5** of this course.



$$\longrightarrow \quad \psi(x)$$

Towards a Quantum Atomic Model

- Atomic spectra
  - A **clue** to atomic structure
  - **Discrete frequencies** imply discrete (i.e. non-continuous) energy states of atom.

$$\frac{1}{\lambda} = R_H \left(\frac{1}{m^2} - \frac{1}{n^2} \right)$$

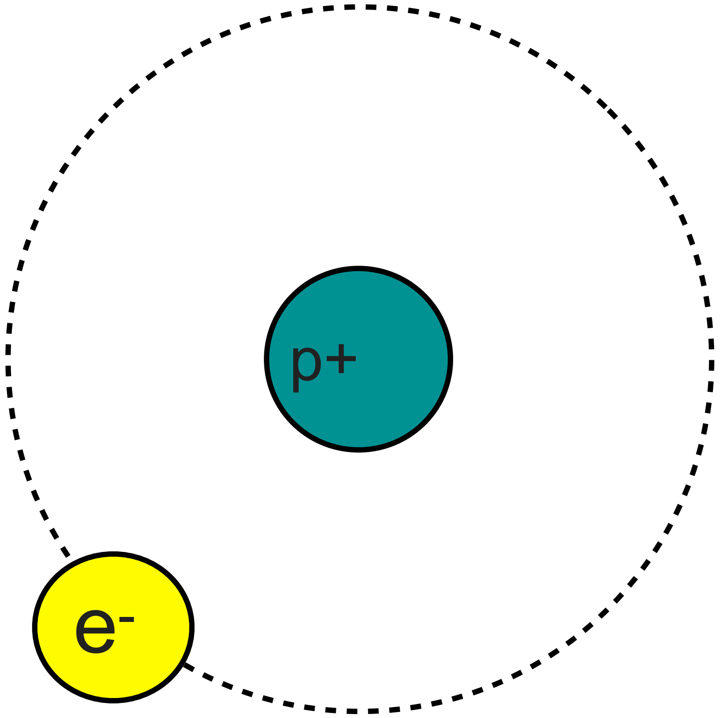
Towards a Quantum Atomic Model

- The Bohr model
  - **Discrete energies** put in "by hand" via angular momentum rule.
  - **Energies** match **Rydberg formula**

Niels Bohr

$$l = mvr = \hbar n = \frac{h}{2\pi} n$$

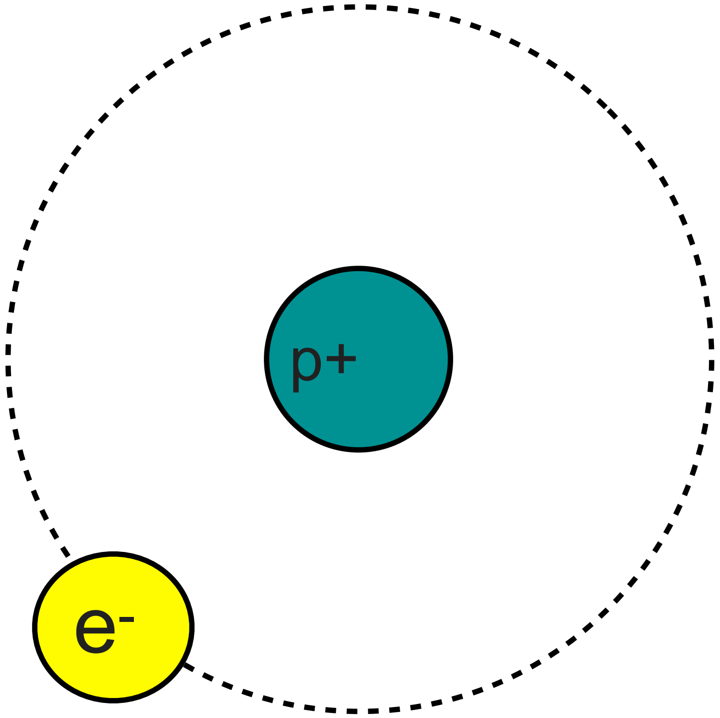
$$E_n = -\left(\frac{1}{2}\frac{1}{4\pi\epsilon_0}\frac{e^2}{a_0}\right)\frac{1}{n^2} = -\frac{hcR_H}{n^2}$$



Towards a Quantum Atomic Model

- Problems with the Bohr model
  - No underlying **physical theory** (incompatible with classical E-M.)
  - Not able to predict **finer details** of spectra for more complicated atoms (even with modifications).
  - Does not include **wave-like** properties of the electron.
  - We know electrons must be represented by **wavefunctions**, not classical orbits.

Niels Bohr



Outline - Part 5 - Energy in Quantum Mechanics

– In this part we will
  - Introduce the **Time-independent Schrödinger Equation**
  - which governs **states of fixed energy** in quantum mechanics.
  - Study examples (**free-particle**, **infinite square well**, **finite well**, **barriers**, **tunnelling**).
  - See quantitatively how the TISE predicts the **spectrum** of **Hydrogen** and other atoms.

Erwin Schrödinger

Today's lecture

– Today we will
  - Introduce the **Time-independent Schrödinger Equation**
  - which governs **states of fixed energy** in quantum mechanics.
  - Introduce two very important examples (**free-particle**, **infinite square well**)

Erwin Schrödinger

Time-independent Schrödinger Equation

Erwin Schrödinger

- What **properties** will determine the wave-functions of the electron in the Hydrogen atom?
- Schrödinger convinced that **energy** was the key.
- 1925 - He proposed an equation - the **Time-independent Schrödinger Equation (TISE).**
- The **TISE** predicts
  - allowed **energies**,
  - and the **wavefunctions** associated with those energies,
- for a **very wide range** of physical settings.

Time-independent Schrödinger Equation

- The **TISE** in 1-dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Erwin Schrödinger

- where
  - **m**: mass of the particle
  - **E**: energy of the particle
  - **V(x)**: The potential energy at position ***x***.

Time-independent Schrödinger Equation

- The **TISE** in 1-dimension:

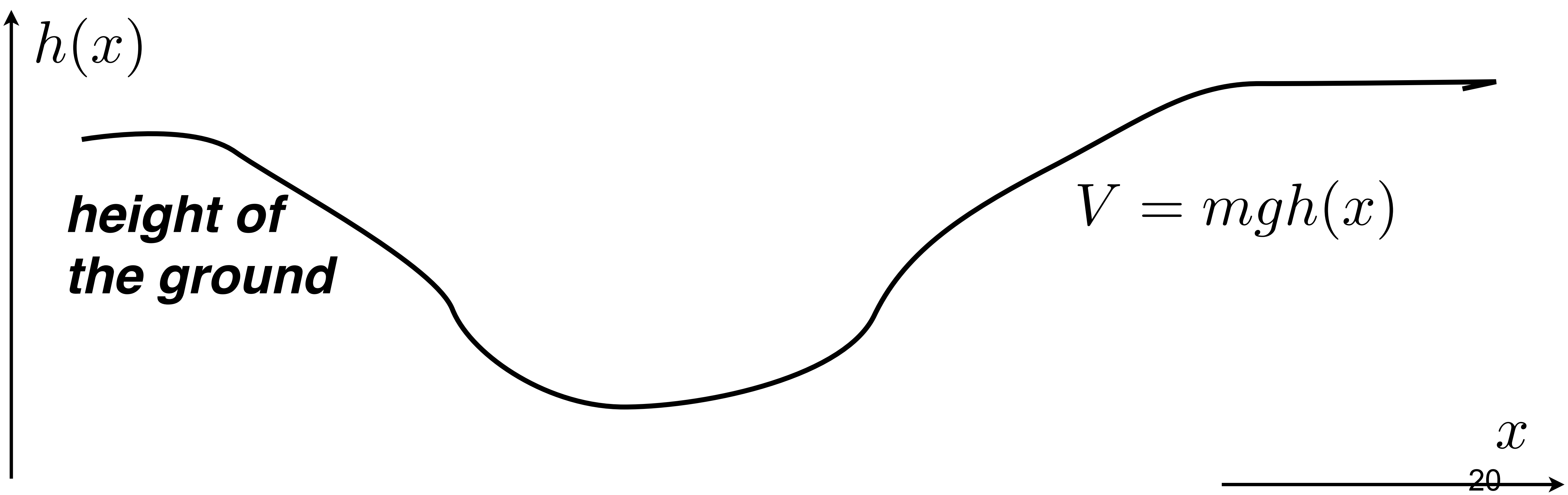
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

Erwin Schrödinger

  - This is a **2nd order differential equation**.
  - When we **solve** it, we recover
    - the allowed **energies E**,
    - and the corresponding **wavefunctions ψ(x).**
- We will solve this equation in several contexts in this course.

Potential Energy

- The term V(x) is **potential energy (**or just **potential).**
- This makes the **TISE extremely flexible.**
- **Many** physical situations can be described in terms of **potential energy**.
- E.g. **gravitational potential**



Poll

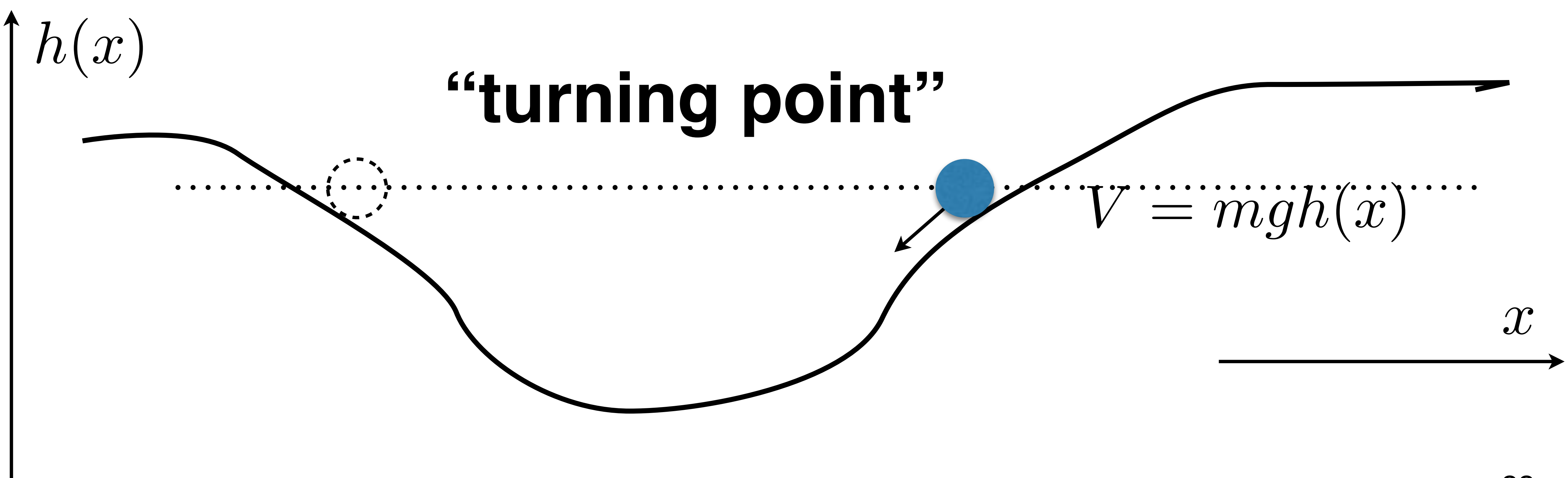
- Have you studied **potential energy** before in classical mechanics?
  - 1. Yes
  - 2. No

- Good treatment: Jewett and Serway - part 1.7

Potential Energy

- In classical mechanics we can compute a particles evolution, from **initial conditions** and the **potential**.
- E.g. if we **release** a stationary particle in a potential we can compute its motion (neglecting friction) via energy conservation.

$$E_{\text{total}} = \frac{p^2}{2m} + V(x)$$



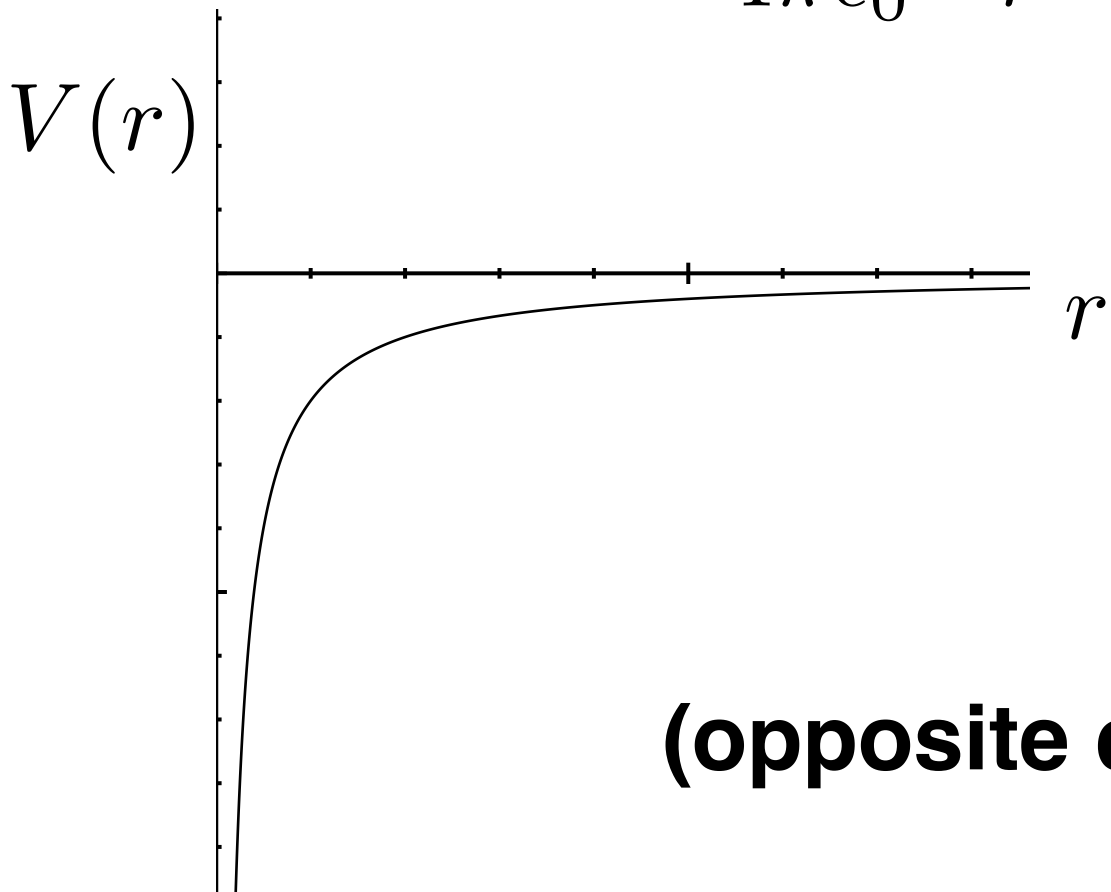
Coulomb Potential

- Potential can be used to describe any conservative **force**.
- Coulomb's law:

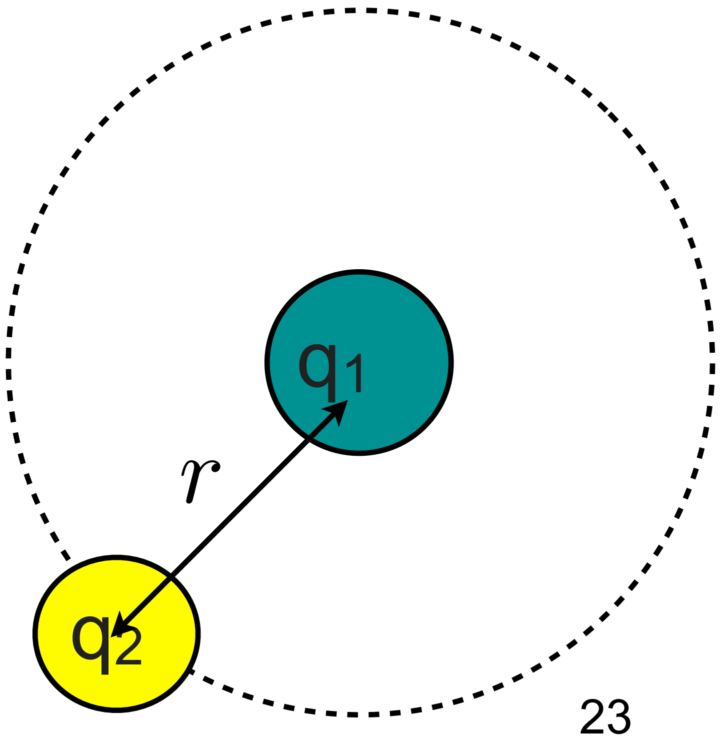
$$|F(r)| = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r^2}$$

can be formulated in terms of potential energy

$$V(r) = \frac{1}{4\pi\epsilon_0}\frac{q_1 q_2}{r} \qquad |F(r)| = \left|\frac{dV}{dr}\right|$$



(opposite charges)



Time-independent Schrödinger Equation

- The **TISE** in 1-dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Erwin Schrödinger

  – The TISE may be used for to study any **potential energy** problem.
  – Hence it has wide applicability.
  – Notice the similarity in structure between the TISE and the classical mechanics equation:

$$\frac{p^2}{2m} + V(x) = E_{\text{total}}$$

Solving the TISE - Free particle

- When there is no potential (**V(x)=0**) we say that the particle is “**free**”.
- The **TISE** for a **free particle** is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

- This equation should look familiar!
- Same form as **simple harmonic motion** in classical mechanics.

$$m\frac{d^2x}{dt^2} = -kx$$

- We solve it in the same way:

Poll

- Have you studied **simple harmonic motion** before in classical mechanics?
  - 1. Yes
  - 2. No

- Overview: Jewett and Serway - part 2.1

Hand-written Calculations

Solving the TISE - Free particle

- We saw that **solutions** to the TISE for a free particle:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

- are the **de Broglie-like wavefunctions** we studied before:

$$\psi(x) = A\sin\left(\frac{px}{\hbar}\right)$$

- or more generally:

$$\psi(x) = A\sin\left(\frac{px}{\hbar} + c\right)$$

- where:

$$E = \frac{p^2}{2m}$$

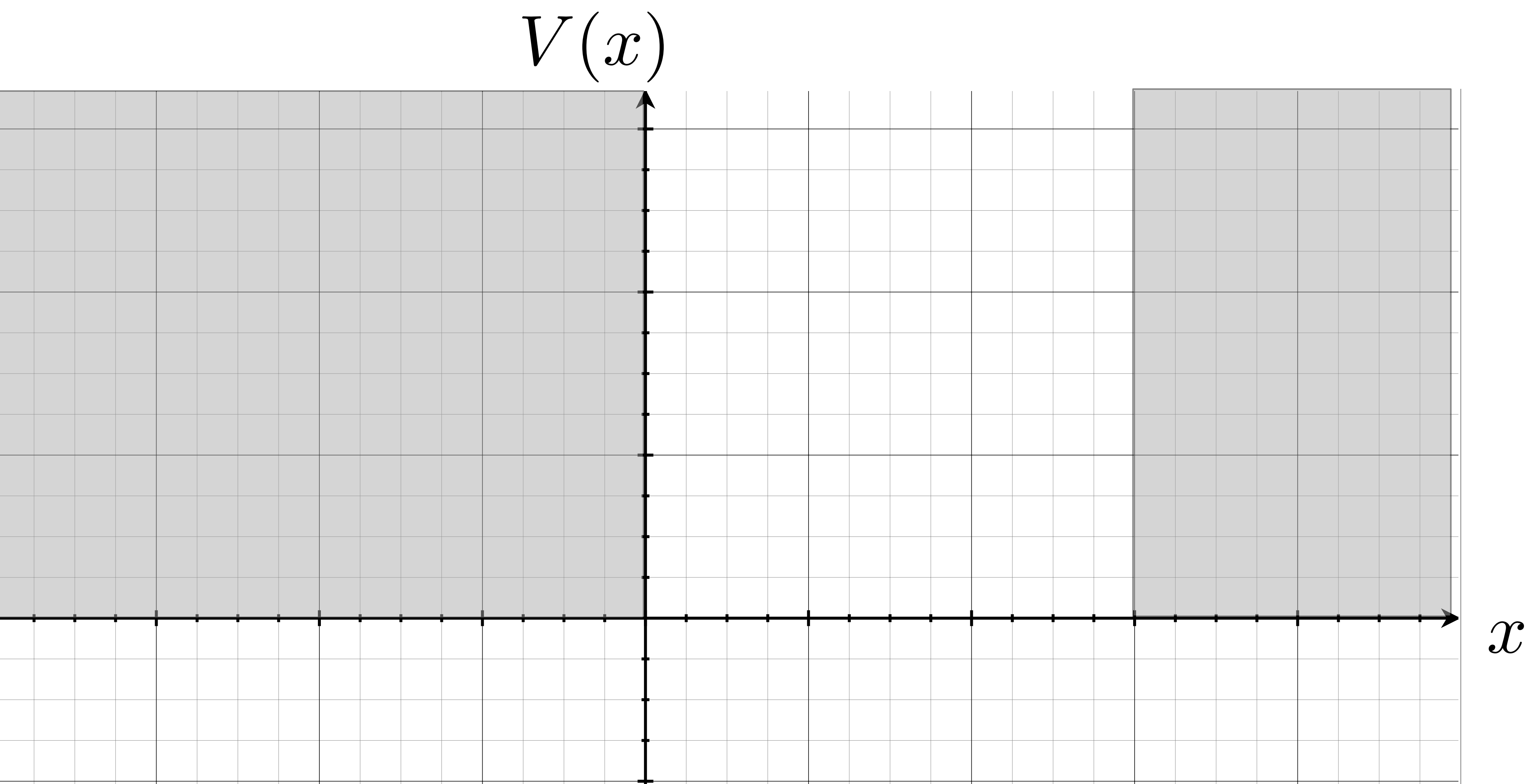
Solving the TISE - Free particle

- This is **consistent** with classical **mechanics**
  - where for a **free particle** (no potential energy) all energy is kinetic energy.

- The **TISE** thus tells us that **these sinusoidal wave-functions** represent states with energy **$E=p^2/2m$**.

Infinite square well

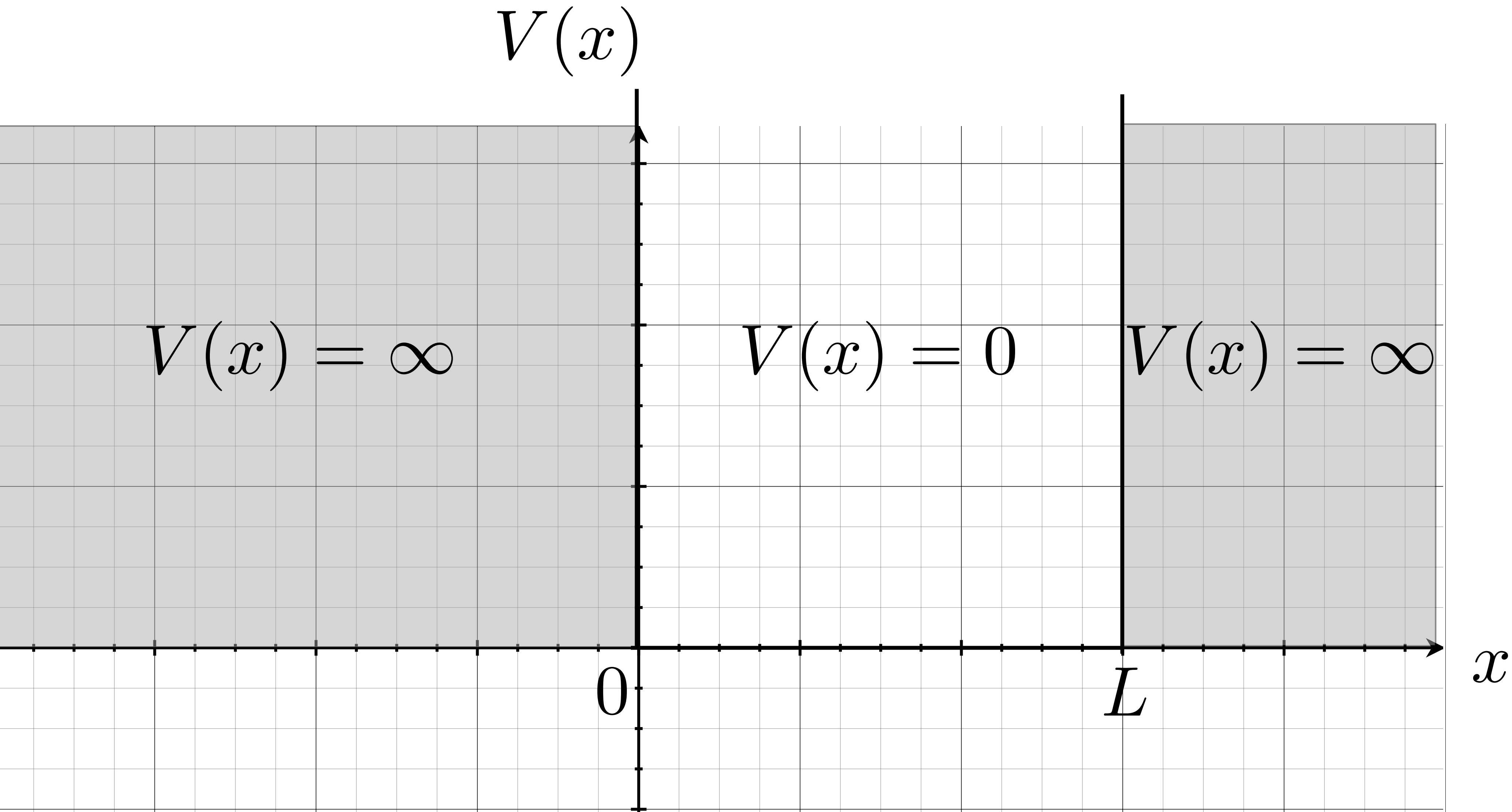
- We have seen that for **free particles** (when V(x)=0) the TISE has **de Broglie-like** wavefunctions as solutions.
- Now we will study our first case with a **non-trivial potential**.
- The **infinite** square well.



Infinite square well

- The **infinite** square well:

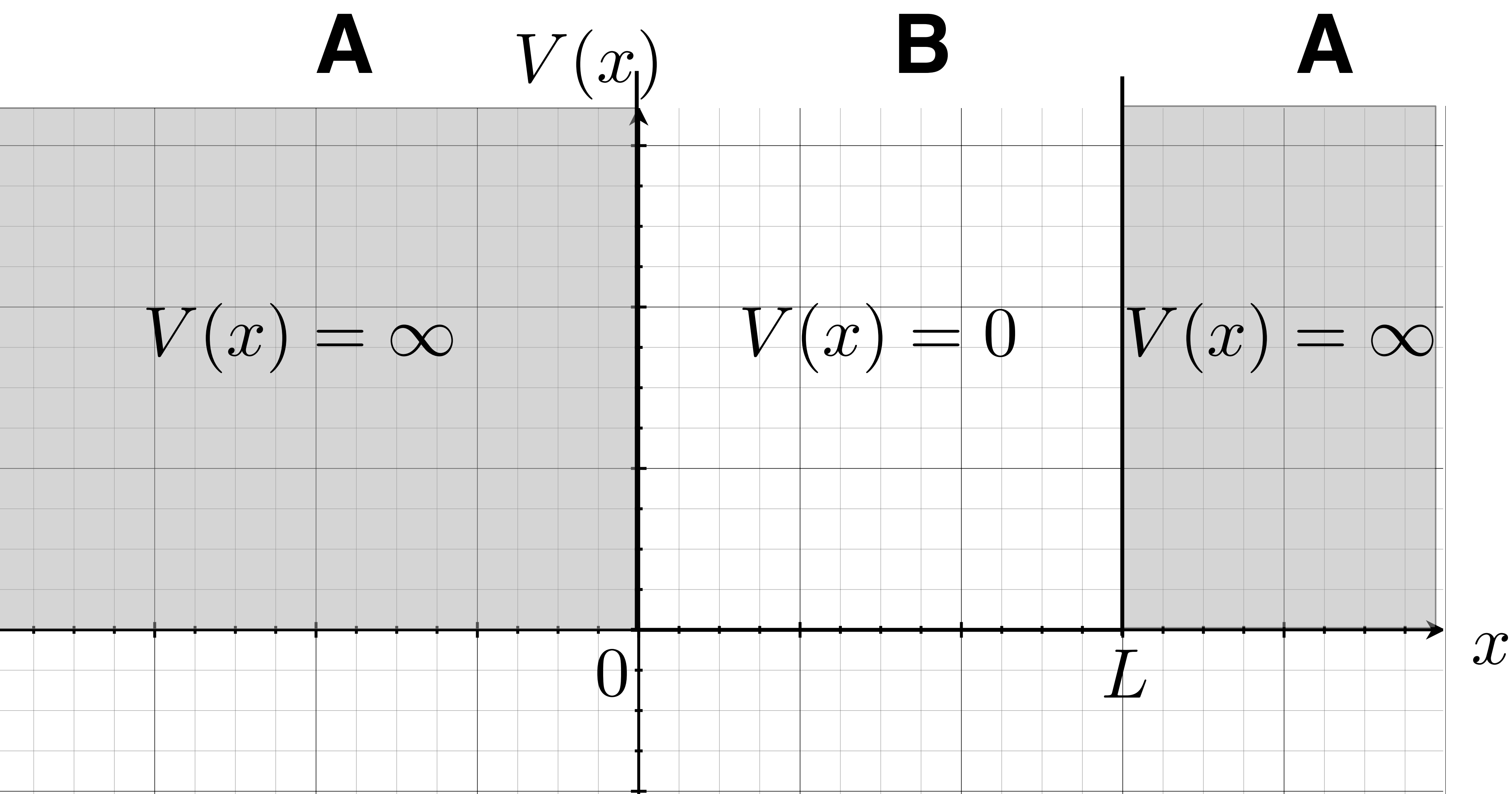
$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{elsewhere} \end{cases}$$



Infinite square well

- Two regions to consider:
  - **A) Infinite potential** - any particle found in this region would have **infinite potential energy** - impossible!
  - Hence, in this region:

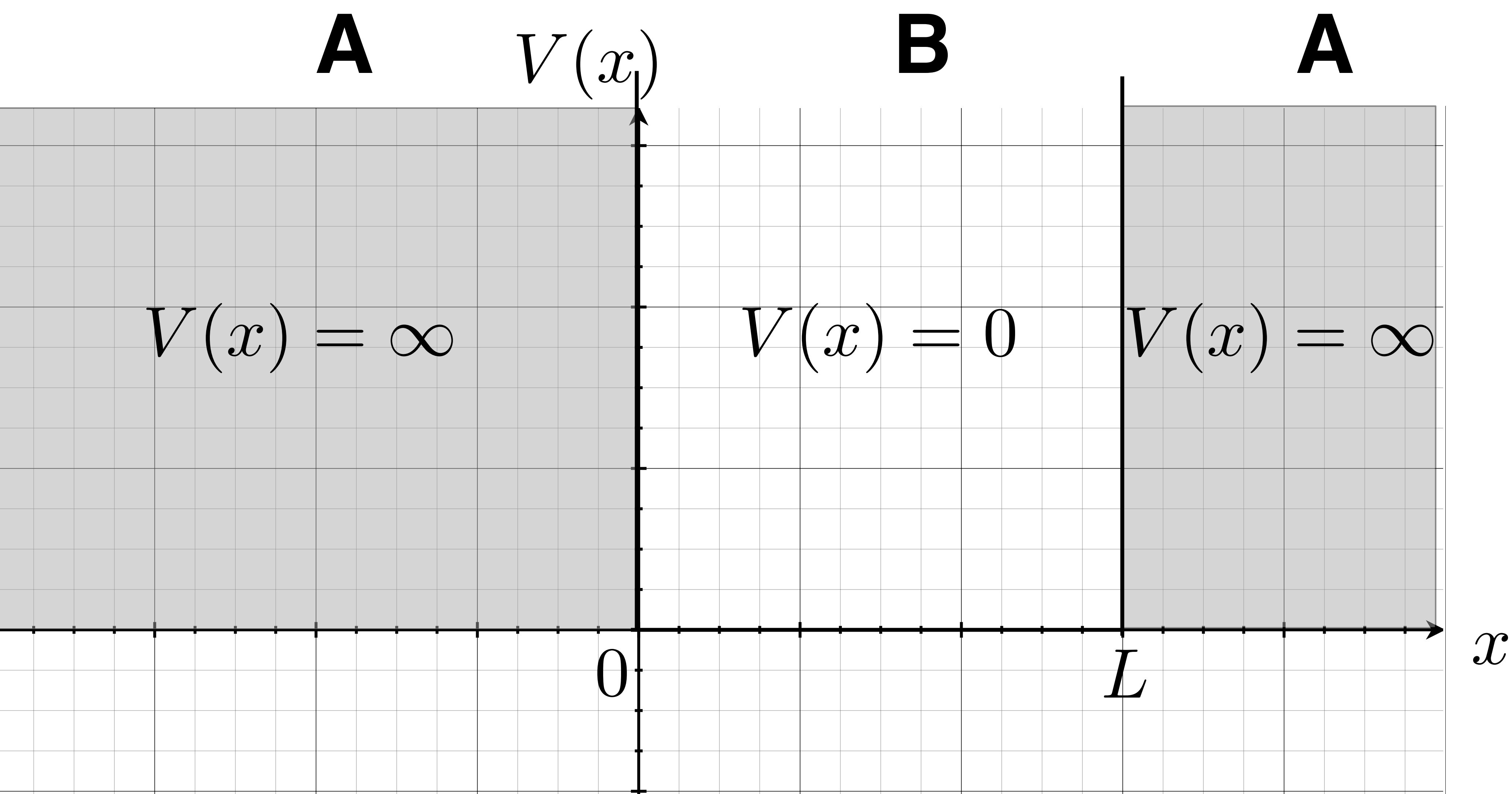
$$\psi_A(x) = 0$$



Infinite square well

- Two regions to consider:
  - **B) Zero potential -** We have already solved TISE with **V(x)=0**.
  - Solutions take the form:

$$\psi_B(x) = a \sin\left(\frac{px}{\hbar} + c\right) \qquad E = \frac{p^2}{2m}$$

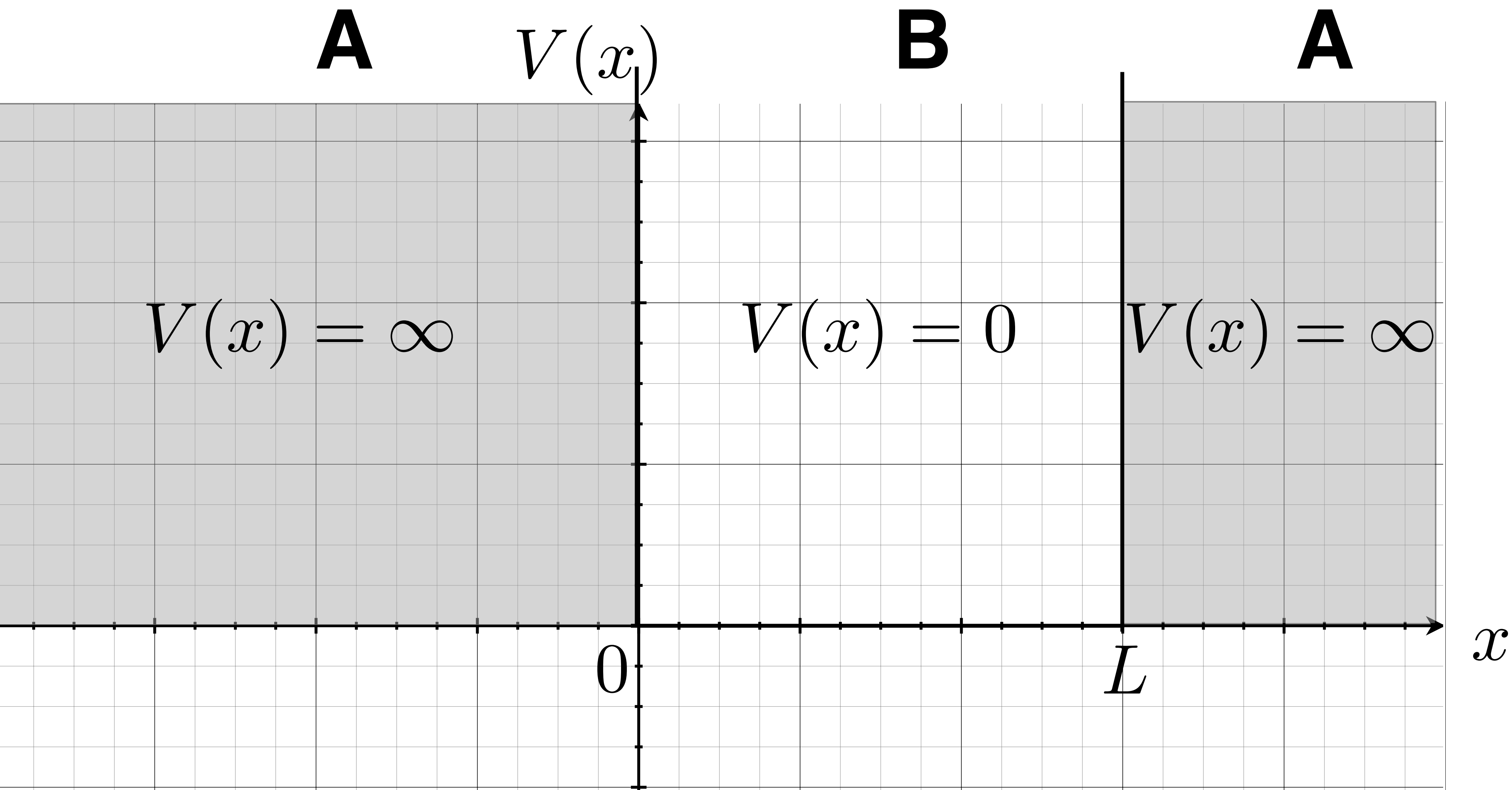


Infinite square well

– Hence we have

$$\psi_A(x) = 0 \qquad\qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = a \sin\left(\frac{px}{\hbar} + c\right) \qquad 0 \leq x \leq L$$



Infinite square well

– Hence we have

$$\psi_A(x) = 0 \qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = a\sin\left(\frac{px}{\hbar} + c\right) \qquad 0 \leq x \leq L$$

– Recall that wavefunctions must be **continuous**.
  - Thus the wavefunctions above must match at the **boundaries.**

– I.e. the following **boundary conditions** must be satisfied:

$$\psi_A(0) = \psi_B(0) \qquad\qquad \psi_A(L) = \psi_B(L)$$

Hand-written Calculations

Infinite square well

- Imposing the boundary conditions leads to the following wave-function in region B.

$$\psi_B(x) = a\sin\left(\frac{n\pi x}{L}\right)$$

- where **n** is an integer.
- If **n = 0, ψ(x)=0** everywhere, so we will discount the **n = 0** solution.
- We can also discount negative integers, since

$$\sin\left(\frac{(-n)\pi x}{L}\right) = -\sin\left(\frac{n\pi x}{L}\right)$$

and we can absorb this minus sign in the, yet to be determined, constant **a**.

Infinite square well

- So the wave-functions in region B for the infinite square well take the form:

$$\psi_B(x) = a\sin\left(\frac{n\pi x}{L}\right)$$

- where **n** = 1, 2, 3, 4…
- We can now use the **TISE** to calculate the **energies** of these wave-functions.

Hand-written Calculations

Infinite square well

- So the wave-functions in region B for the infinite square well take the form:

$$\psi_B(x) = a \sin\left(\frac{n\pi x}{L}\right)$$

- where **n** = 1, 2, 3, 4…
- We can now use the **TISE** to calculate the **energies** of these wave-functions and find:

$$E_n = \frac{h^2}{8mL^2} n^2$$

- The energies only take **discrete values** - the energy is **quantised**.
- Unlike in the Bohr model, where quantisation was put in by hand, this **quantisation** has **emerged** from the requirement of a **continuous** wavefunction - the **boundary conditions**.

Infinite square well

- We have not yet checked whether the wavefunctions are normalisable or normalised.

$$\psi_A(x) = 0 \qquad\qquad x \leq 0 \quad x \geq L$$

$$\psi_B(x) = a \sin\left(\frac{n\pi x}{L}\right) \qquad\qquad 0 \leq x \leq L$$

- Recall, all physical wavefunctions must satisfy:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

- Let us verify that our wave-functions can be **normalised**.

Hand-written Calculations

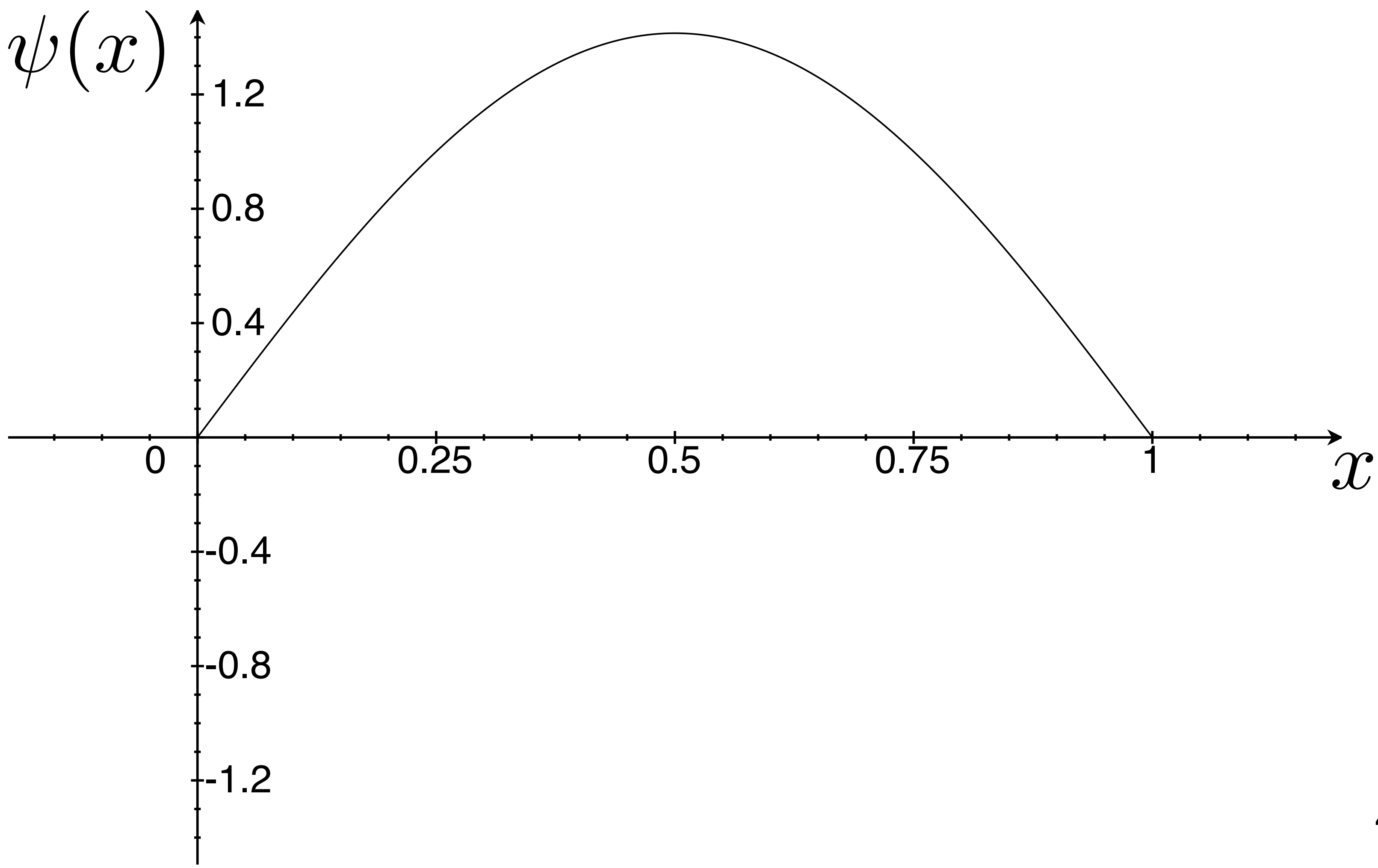
Infinite square well

- The normalised wave-functions are:

$$\psi_A(x) = 0 \qquad\qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad 0 \leq x \leq L$$

- E.g. **n=1 L=1,**



Infinite square well

- The normalised wave-functions are:

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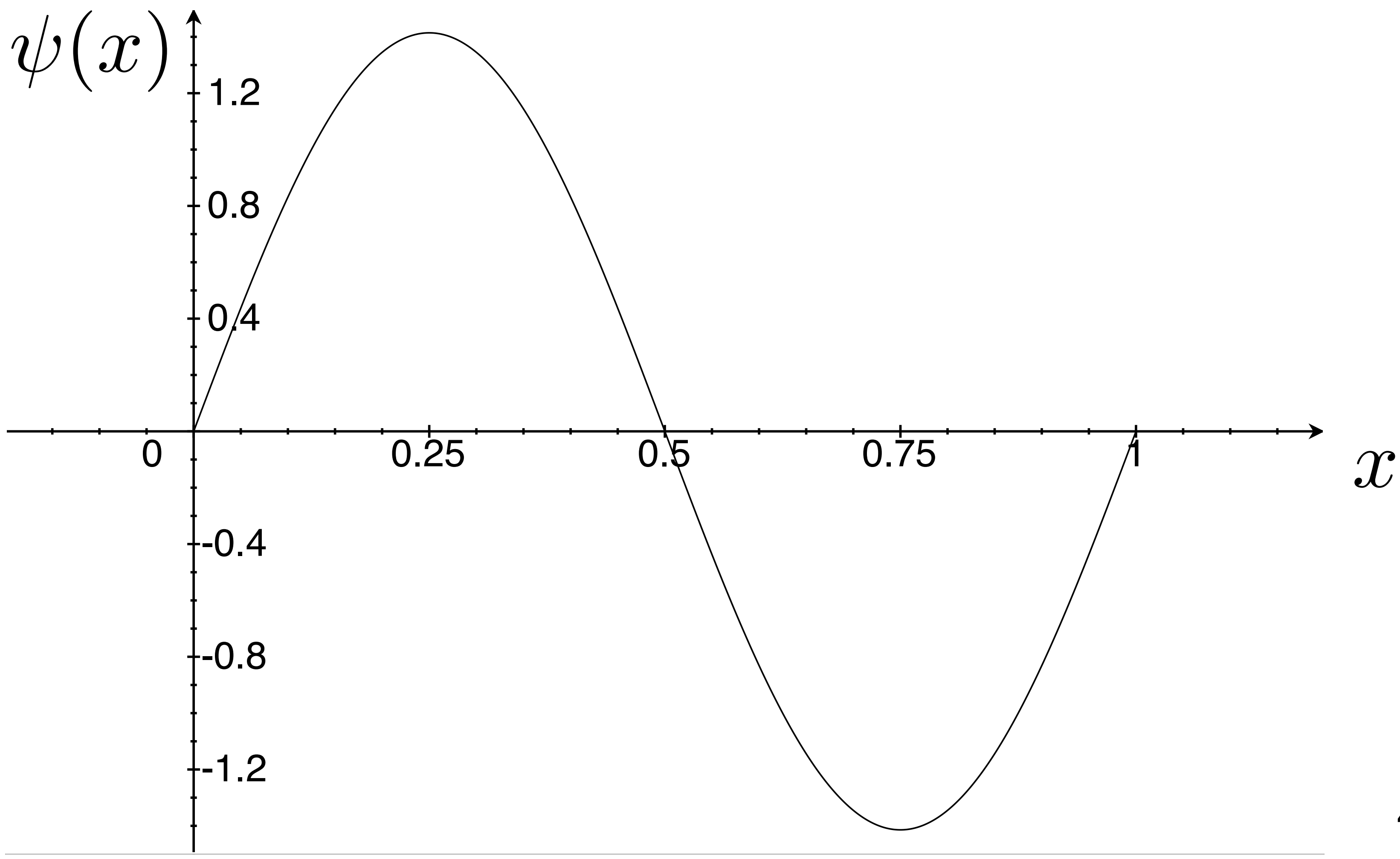
- E.g. **n=2, L=1**



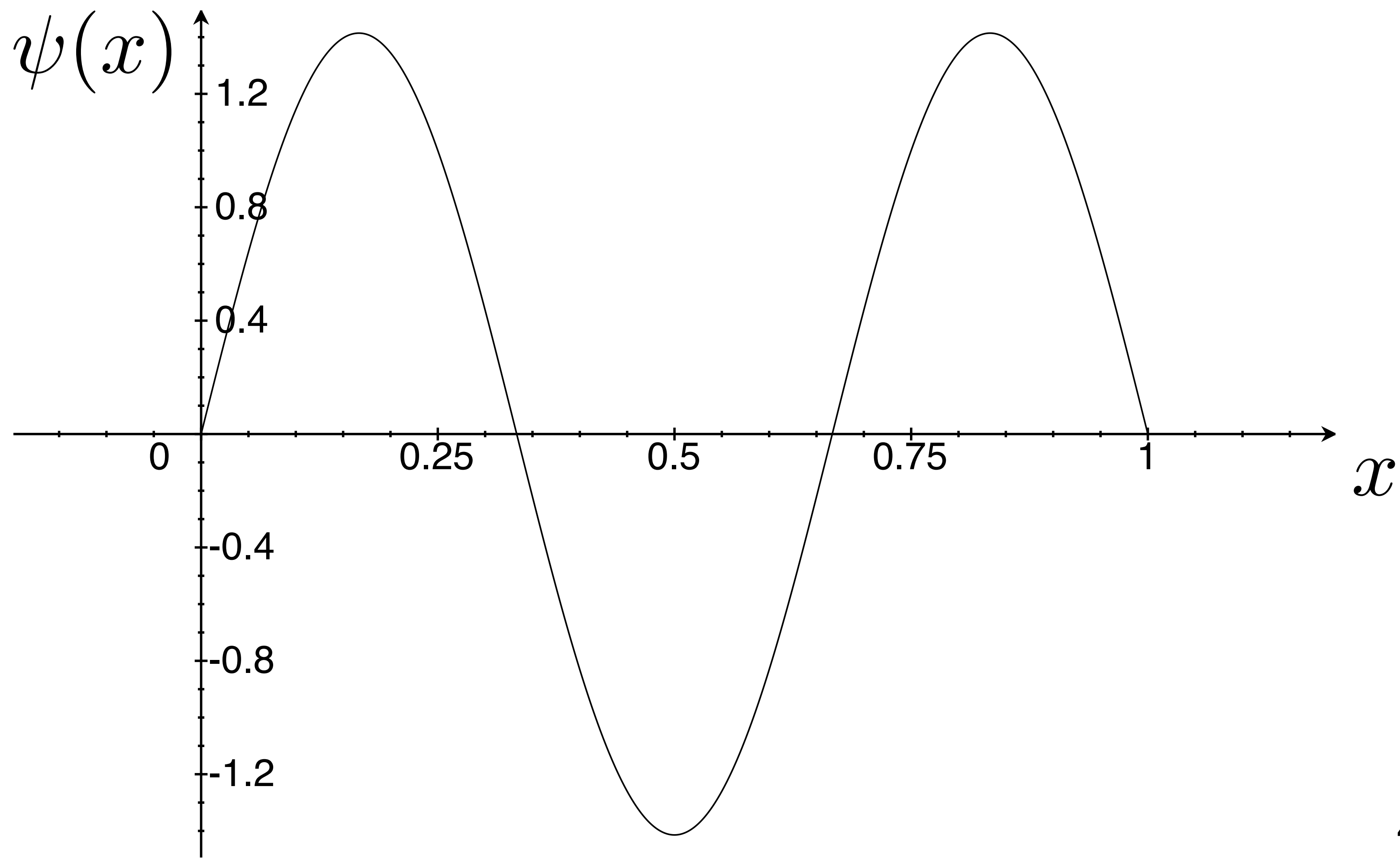
Infinite square well

- The normalised wave-functions are:

$$\psi_A(x) = 0 \qquad\qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad 0 \leq x \leq L$$

- E.g. **n=3, L=1**



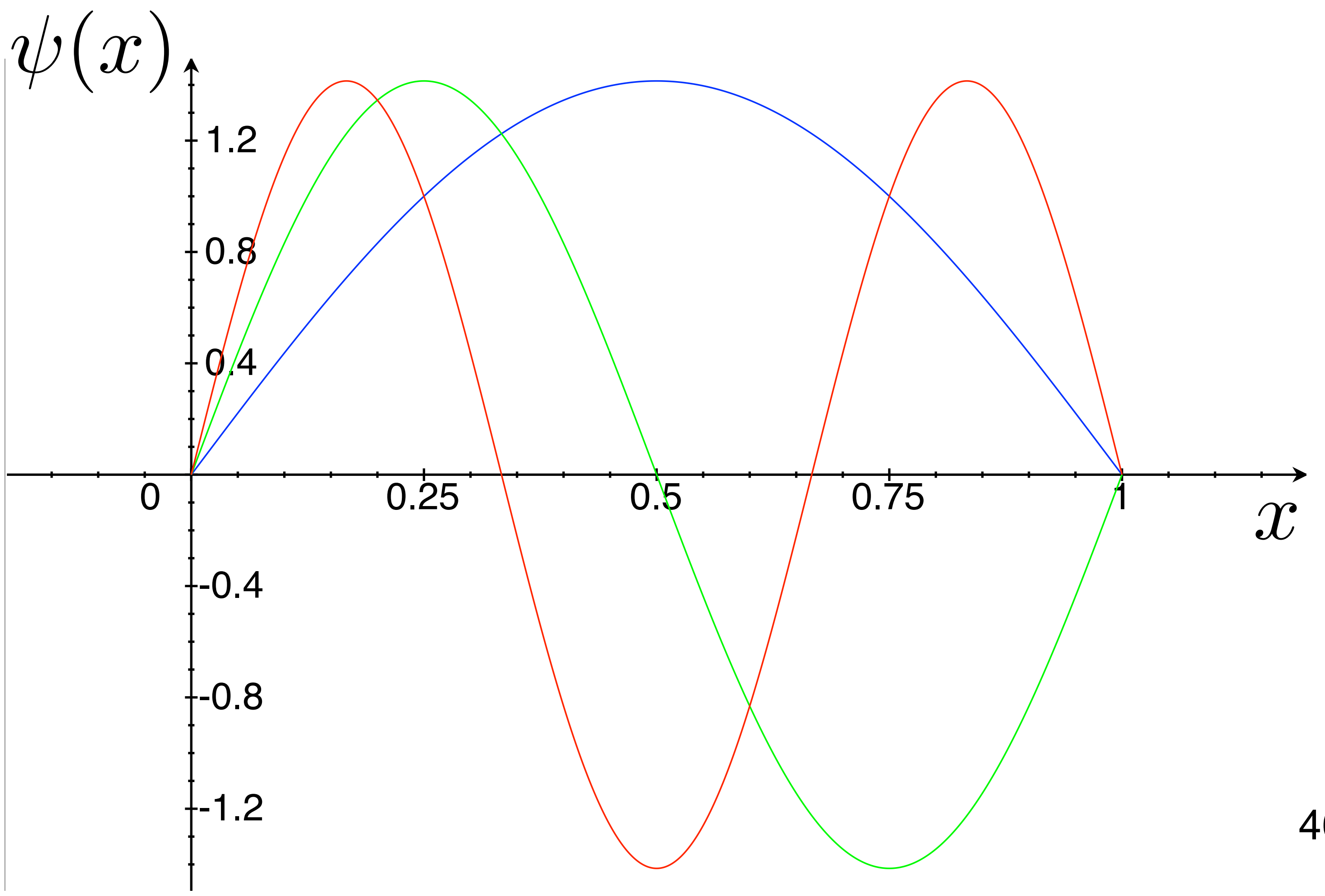
Infinite square well

- The normalised wave-functions are:

$$\psi_A(x) = 0 \qquad x \leq 0 \quad x \geq L$$

$$\psi_B(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad 0 \leq x \leq L$$

- E.g. **n=1,2,3 L=1**



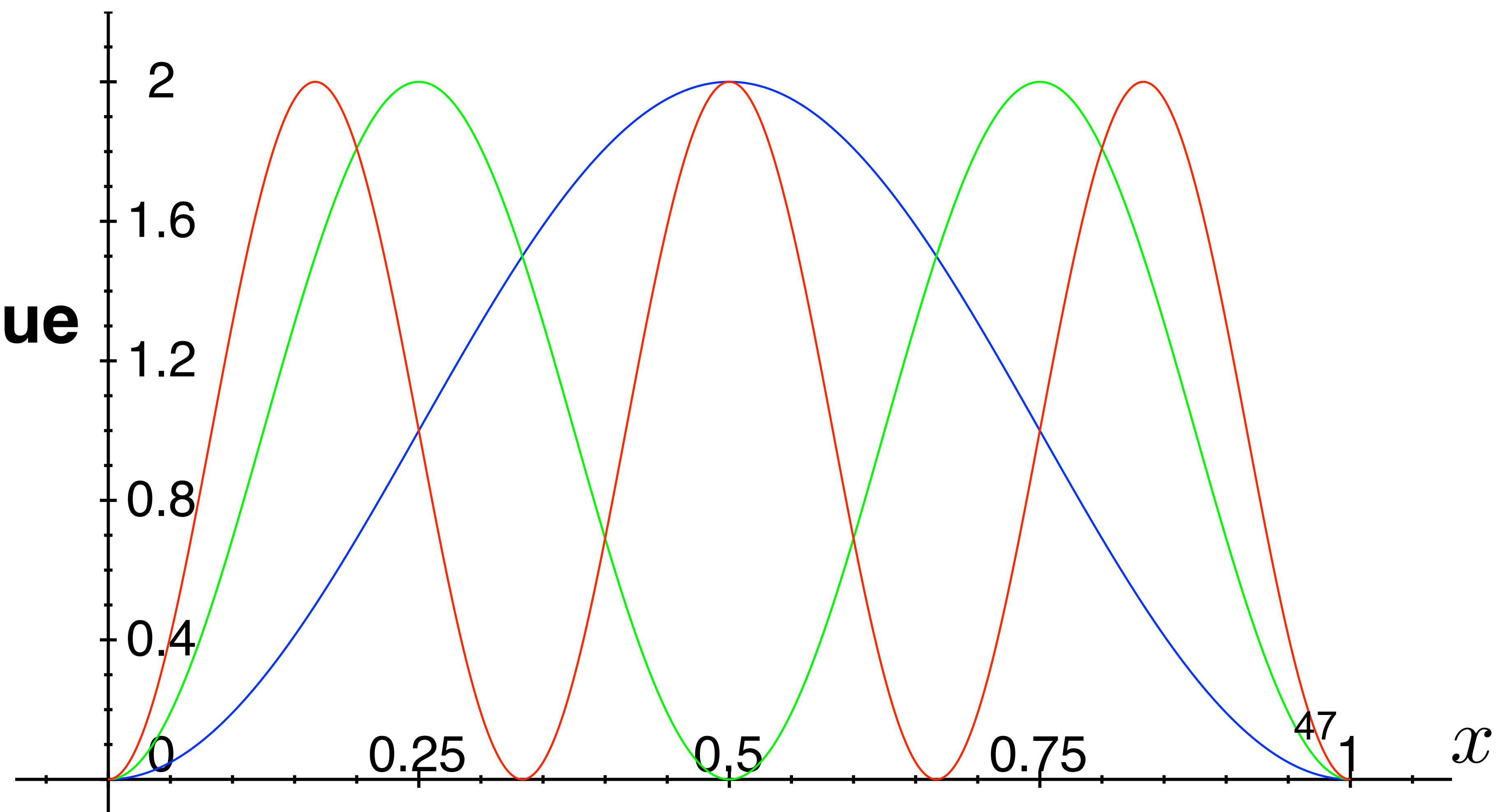
Infinite square well

- The corresponding **probability density** for position:

$$\rho(x) = 0 \qquad\qquad x \leq 0 \quad x \geq L$$

$$\rho(x) = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right) \qquad\qquad 0 \leq x \leq L$$

- E.g. **n=1,2,3**
  L=1,



- **For all values of n, the expectation value of x is:**

$$\langle x \rangle = \frac{L}{2}$$

Infinite square well

- Summary
  - By solving the TISE and applying boundary conditions, we find that the **only allowed energies** for the **infinite square well** are:

$$E_n = \frac{h^2}{8mL^2}n^2$$

  - and the corresponding wave-functions:

$$\psi_A(x) = 0 \qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \qquad 0 \leq x \leq L$$

Infinite square well

- Our solution strategy
  - Solve the TISE in **separate regions** of **constant potential.**
  - Use continuity of wavefunction between region to give us **boundary conditions**.
- This is a **general technique** which we will use often in solving the TISE.
- Before we consider some other examples, we will take a closer look at the **structure** of the TISE.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

Structure of the TISE

– Let us take another look at the **time-independent Schrödinger equation.**

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

– The wavefunction **ψ(x)** appears in every term of the equation.

– As already noted, it has a similar structure to:

$$\frac{p^2}{2m}+V(x)=E_{\text{total}}$$

Differential operators

- You are familiar with writing **derivatives**.
  - E.g. First derivative of $f(x)$: $\dfrac{df(x)}{dx}$
- The mathematical object: $\dfrac{d}{dx}$

  is called a **differential operator**.
- It acts as follows: $$\frac{d}{dx}f(x) = \frac{df(x)}{dx}$$
- Examples of differential operators:

$$\frac{d}{dx} \qquad \frac{d^2}{dt^2} \qquad \frac{d^2}{dxdy}$$

Structure of the TISE

–We can rewrite the TISE in terms of differential operators:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

$$\downarrow$$

–Equations in the form

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

$$\hat{D}\psi(x) = E\psi(x)$$

–are called **eigenvalue equations**.

- where ***E*** is called the **eigenvalue**
- **ψ(x)** is called the **eigenfunction**
- and $\hat{D}$ is any sum of differential operators and functions of ***x***.

Structure of the TISE

- The **Time-independent Schrödinger equation** is an example of an **eigenvalue equation**,
  – where energy **E** is the **eigenvalue**
  – and wavefunction **ψ(x)** is the **eigenfunction**

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x)$$

- As we have seen, the TISE can have **multiple eigenvalues** (the allowed energies), and for each eigenvalue a **different eigenfunction** (the wavefunction for that energy).
- **Eigenvalue equations** play a **central role** in quantum mechanics and you will study them in great detail in your future courses.

Summary of last lecture

- We introduced the **Time-Independent Schrödinger Equation.**

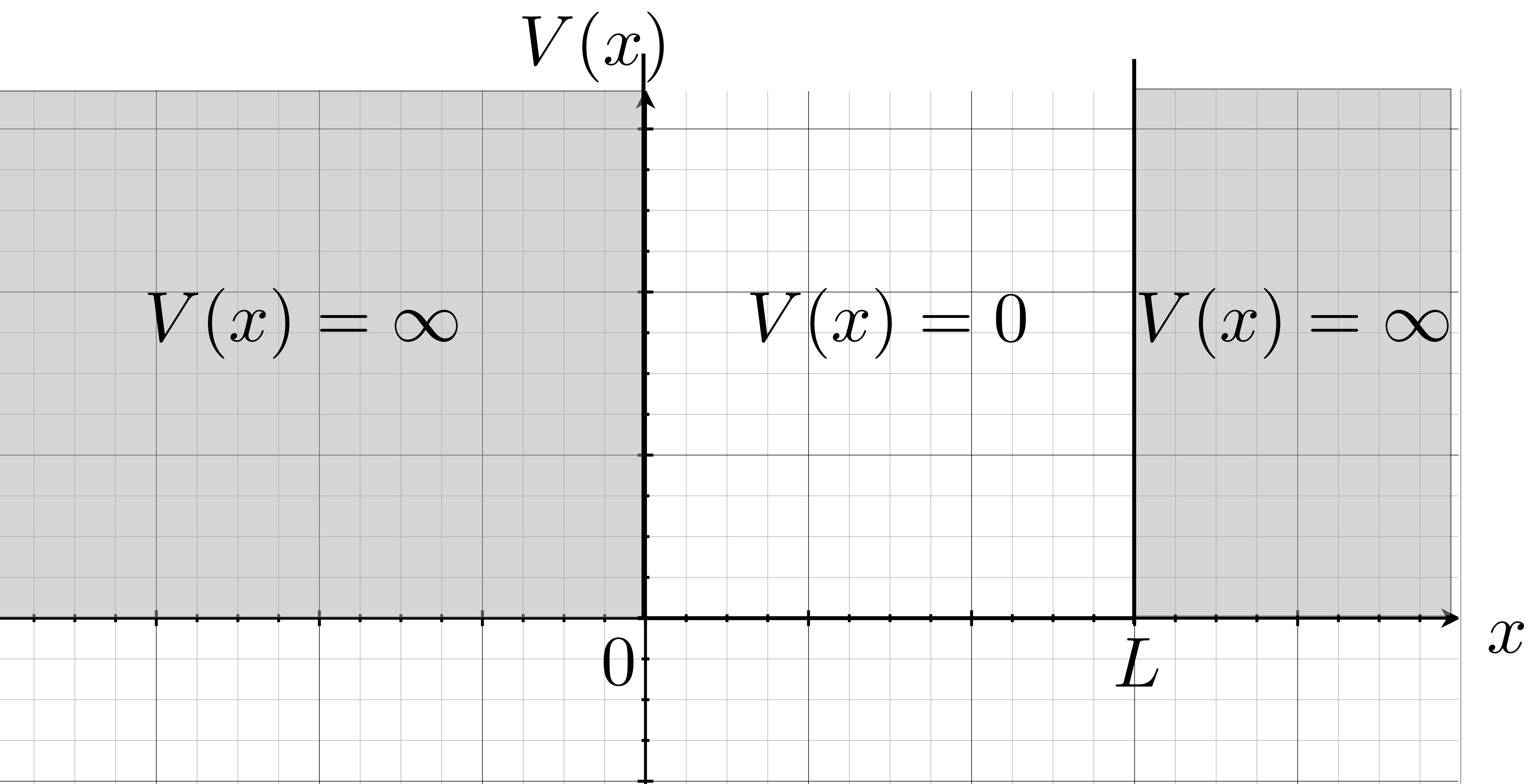
$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

- where
  - **m**: **mass** of the particle
  - **E**: **energy** of the particle
  - **V(x)**: The **potential** energy at position ***x***.
  - **ψ(x):** The particle **wavefunction**.

Infinite square well

- The **infinite** square well:

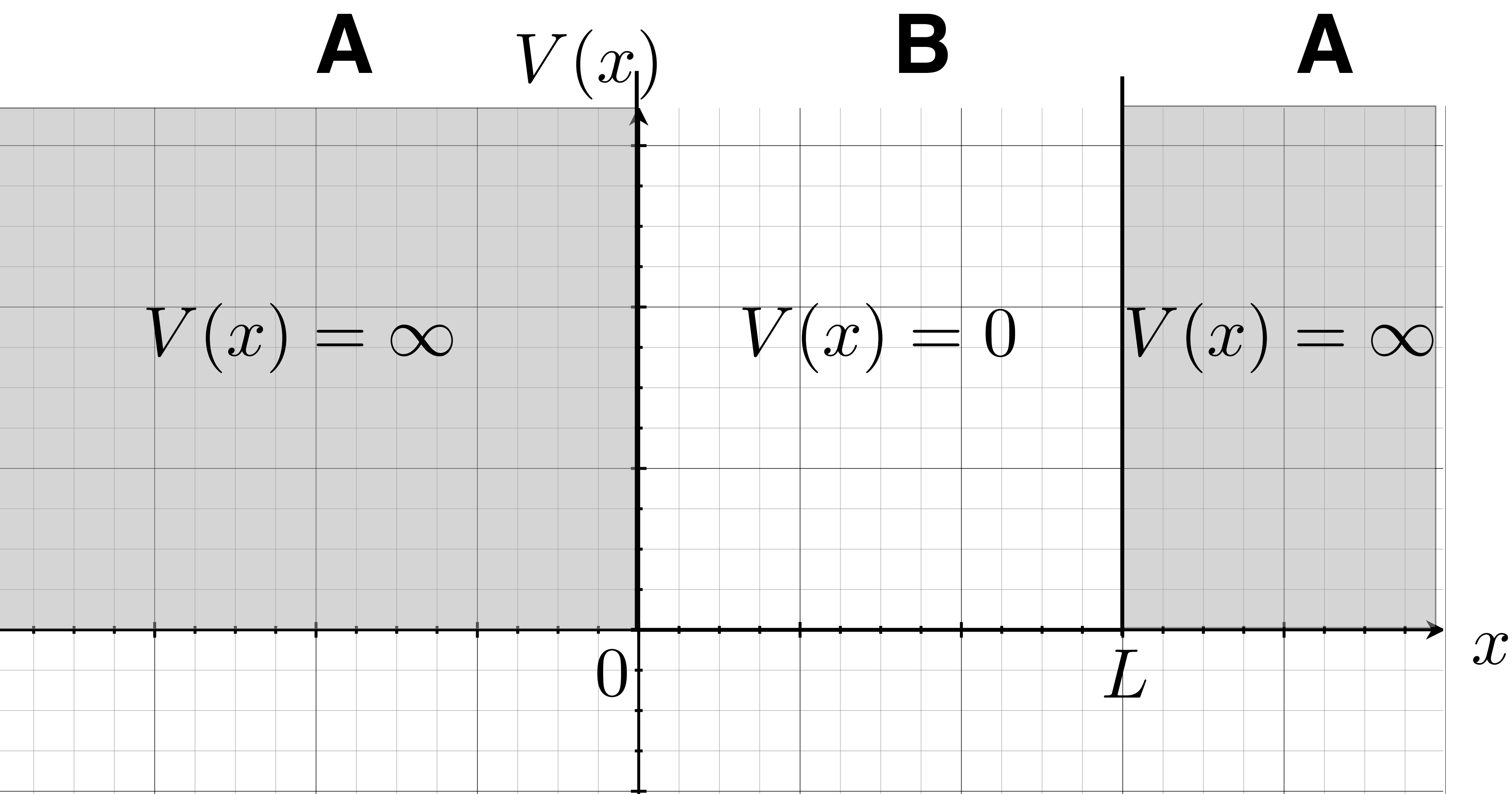
$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{elsewhere} \end{cases}$$



Infinite square well

- Two regions to consider:
  - **B) Zero potential -**
  - Solutions take the form:

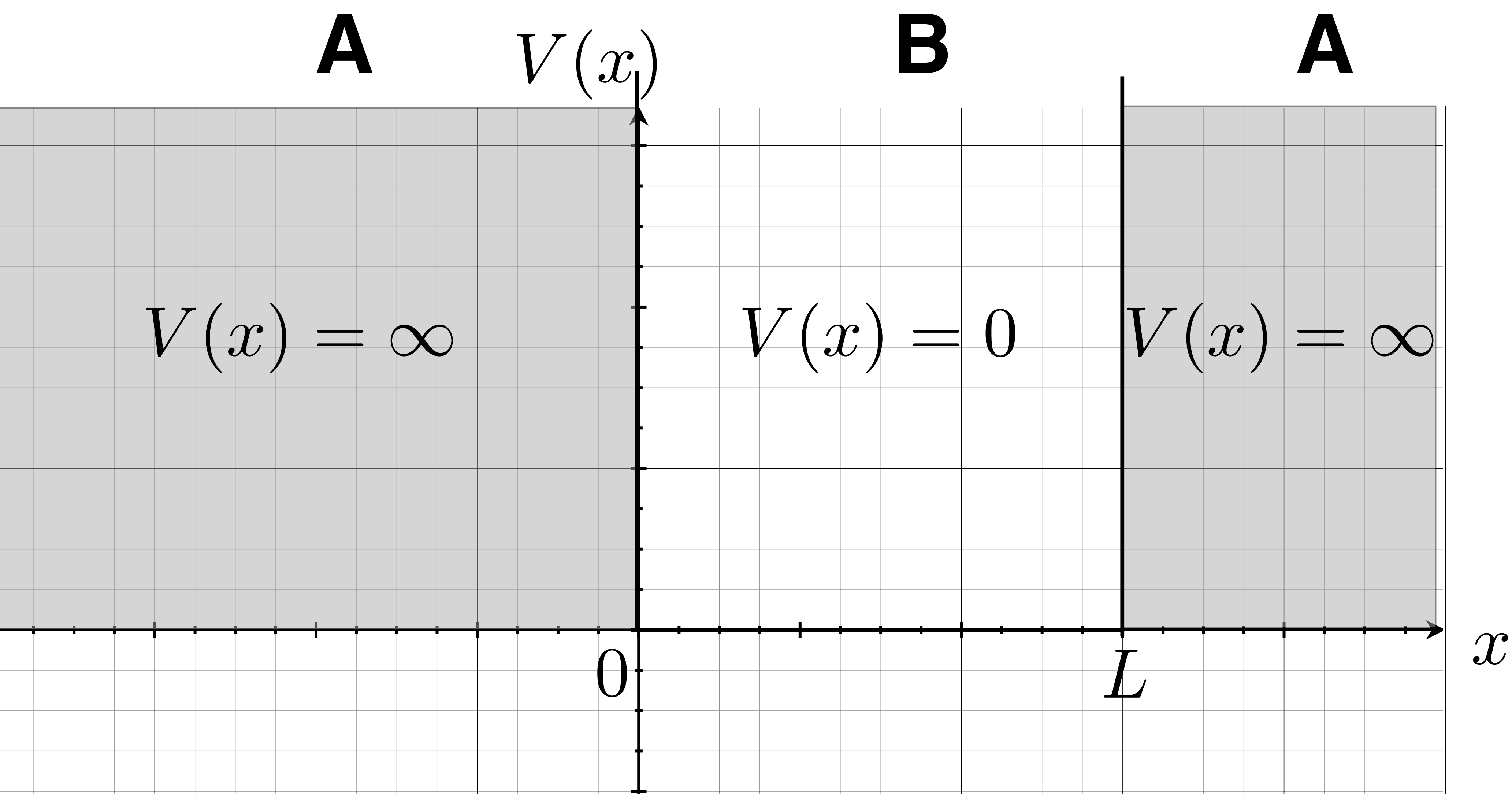
$$\psi_B(x) = a\sin\left(\frac{px}{\hbar} + c\right) \qquad E = \frac{p^2}{2m}$$



Infinite square well

- Two regions to consider:
  - **A) Infinite potential** - any particle found in this region would have **infinite potential energy** - impossible!
  - Hence, in this region:

$$\psi_A(x) = 0$$



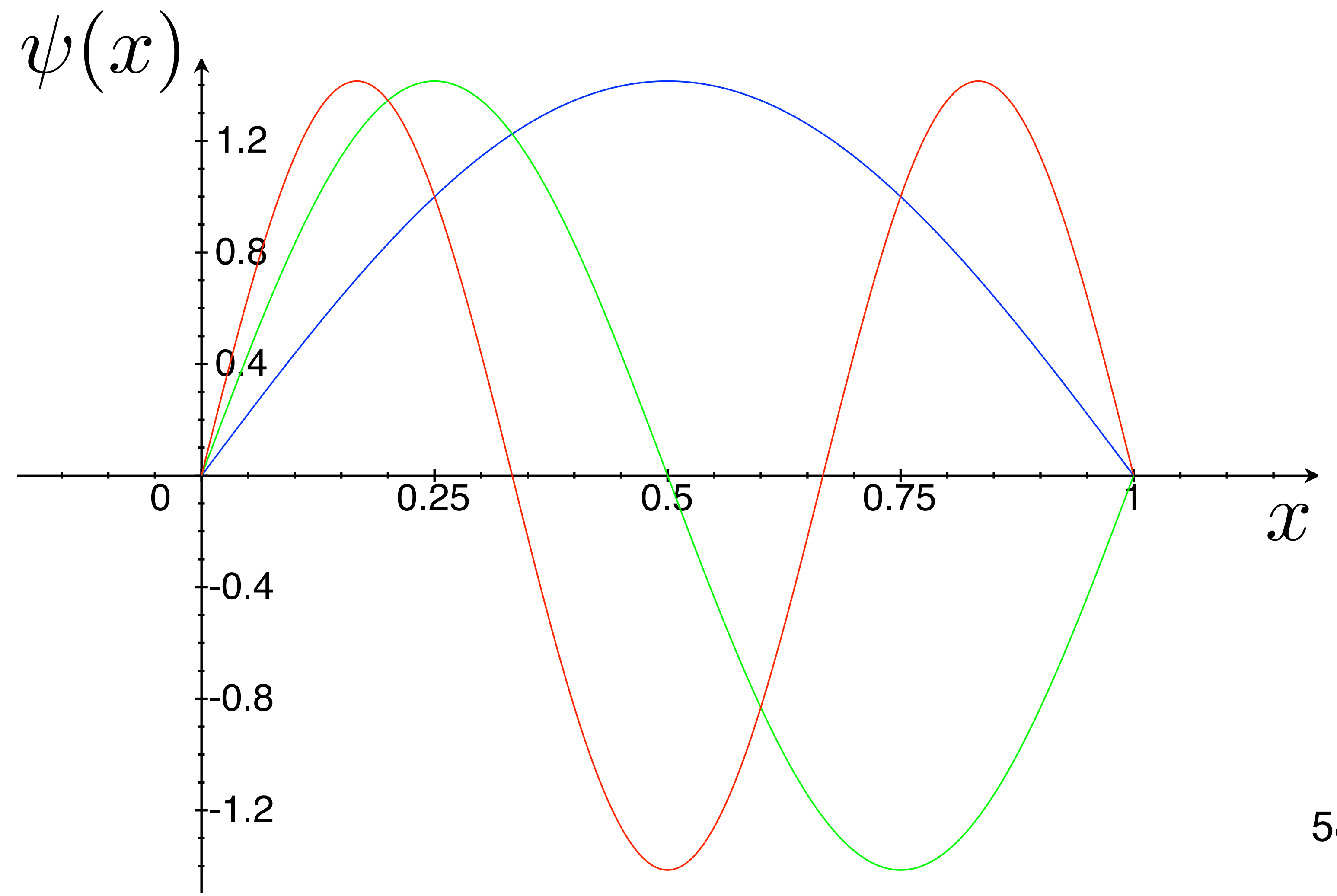
Infinite square well

- Applying **boundary conditions** and **normalising**:

$$\psi_A(x) = 0 \qquad x \leq 0 \quad x \geq L$$

$$\psi_B(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad 0 \leq x \leq L$$

- E.g. **n=1,2,3**
  L=1



Finite square well

- The **infinite square well** is an important first example of solving the TISE.
- In nature, potential energy is usually **finite**.
- We will study the **finite square well**.

Finite square well

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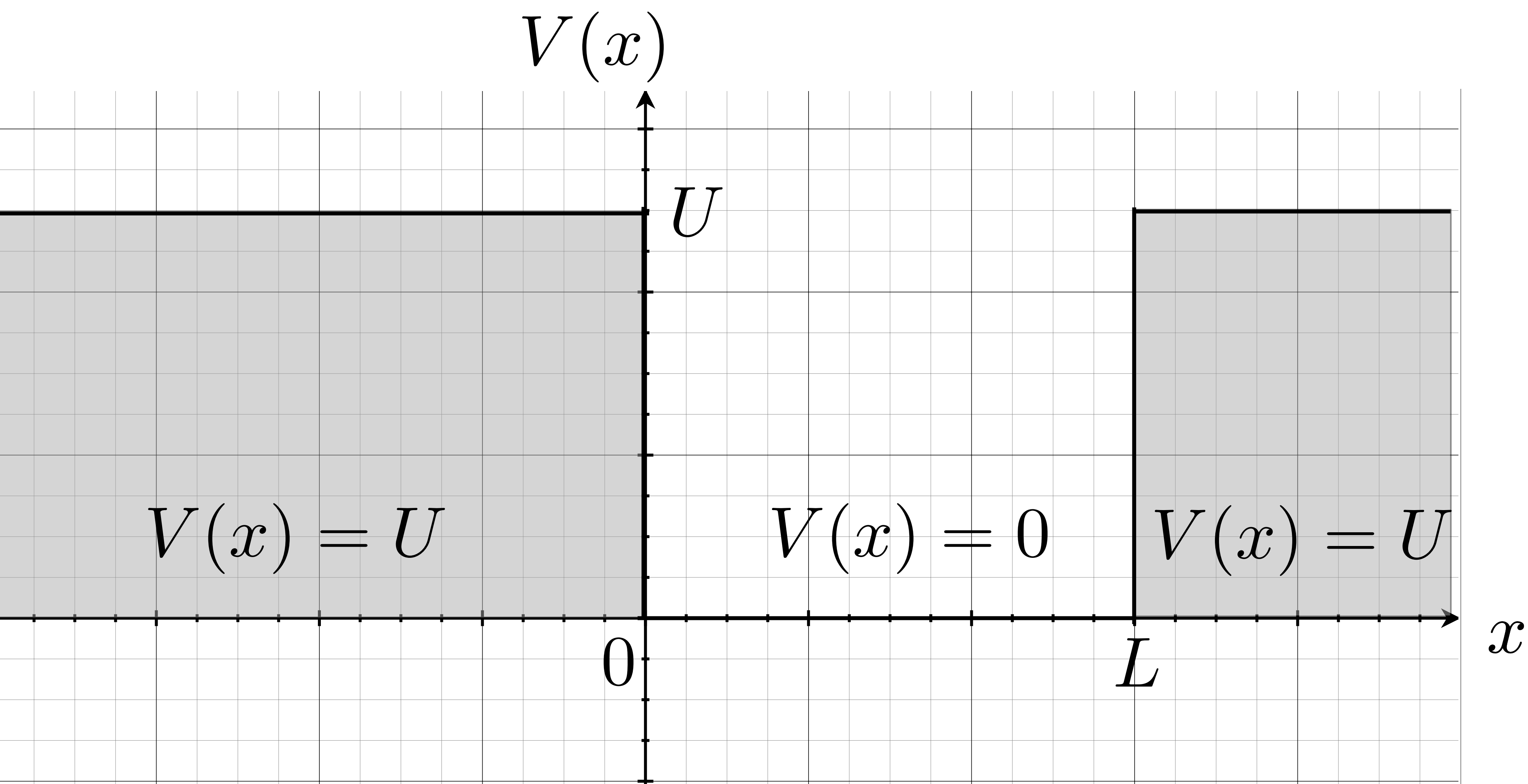
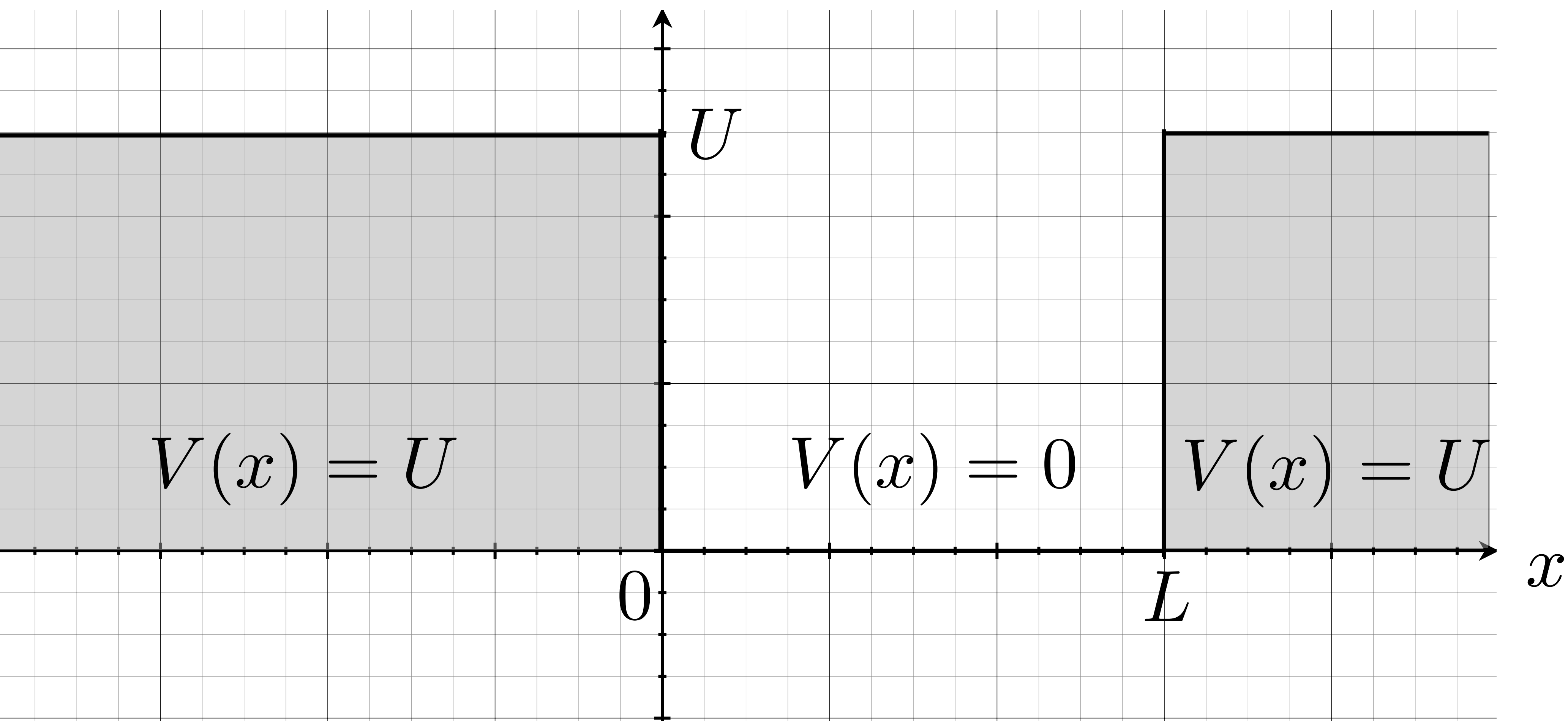


Finite square well

- The potential function for the finite square well is:

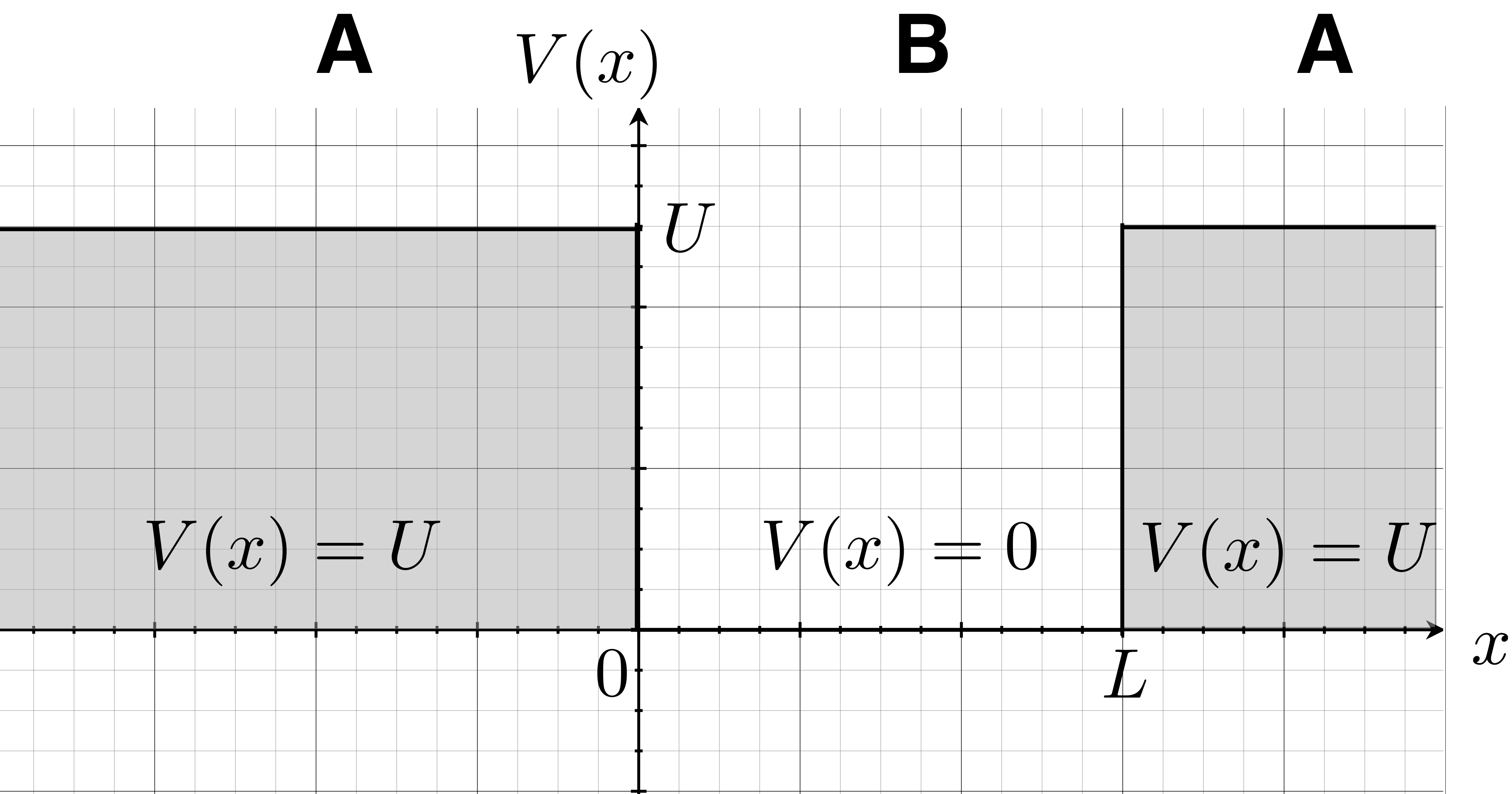
$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ U & \text{elsewhere} \end{cases}$$

$$V(x) \qquad U > 0$$



Finite square well

- To solve the **TISE**, we again split the problem up into **regions**, and then apply **boundary conditions**.
  - **Region A)** where **V(x) = U.**
  - **Region B)** where **V(x) = 0.**



Boundary conditions

- We have seen that wavefunctions must be **continuous**.
- The reason for this is that in a **discontinuous** function, the **gradient**, or **first derivative** is **infinite**.

Boundary conditions

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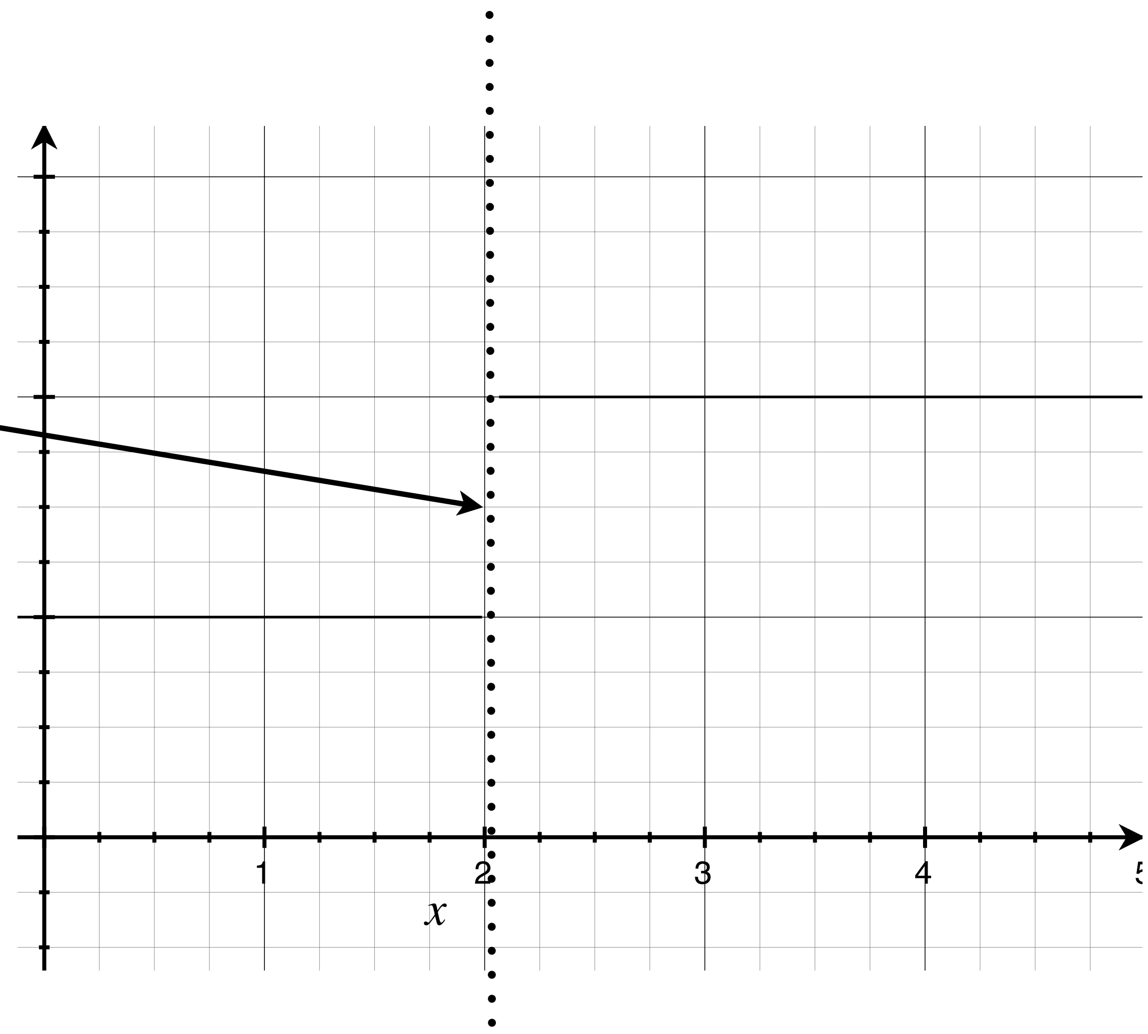
- The reason for this is that in a **discontinuous** function, the **gradient**, or **first derivative** is **infinite**.

Infinite gradient $\frac{\Delta y}{\Delta x}$



$f(x)$ **discontinuous** $\longrightarrow$ $\frac{df(x)}{dx}$ **infinite**

Boundary conditions

- Similarly $\frac{d^2 f(x)}{dx^2}$ is the gradient of $\frac{df(x)}{dx}$

- So

$$\frac{df(x)}{dx} \ \textbf{discontinuous} \longrightarrow \frac{d^2 f(x)}{dx^2} \ \textbf{infinite}$$

similar to

$$f(x) \ \textbf{discontinuous} \longrightarrow \frac{df(x)}{dx} \ \textbf{infinite}$$

Boundary Conditions

– The TISE contains the second derivative of ψ(x):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

– If **energy E** is **finite**, the second derivative cannot be infinite, hence the first derivative of the wave-function must be continuous.

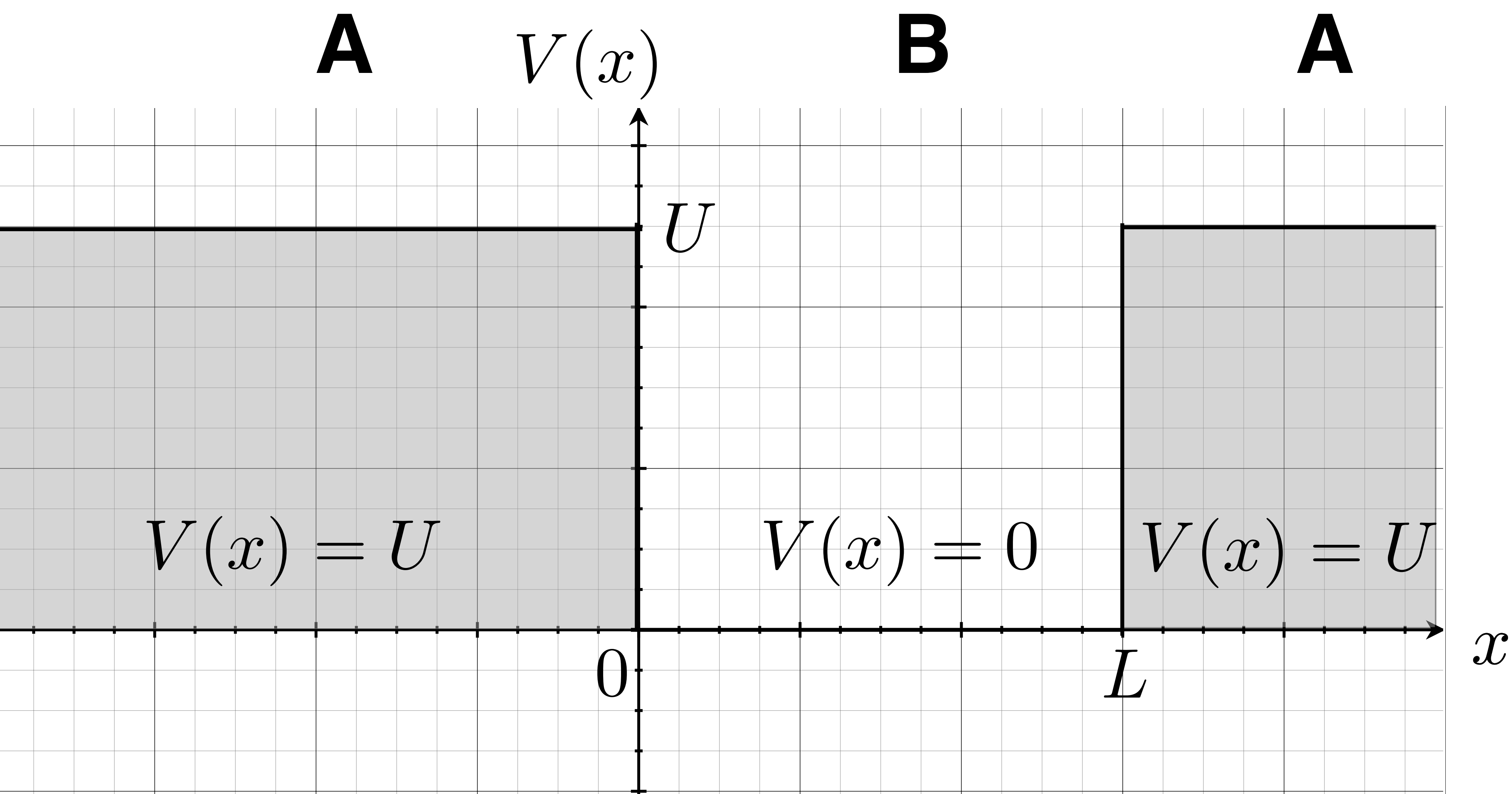
– This gives us an extra continuity condition:

- **ψ(x)** must be **continuous**
- **dψ(x)/dx** must be **continuous**

– This contributes an **additional boundary condition** which **TISE solutions** must satisfy.

Finite square well

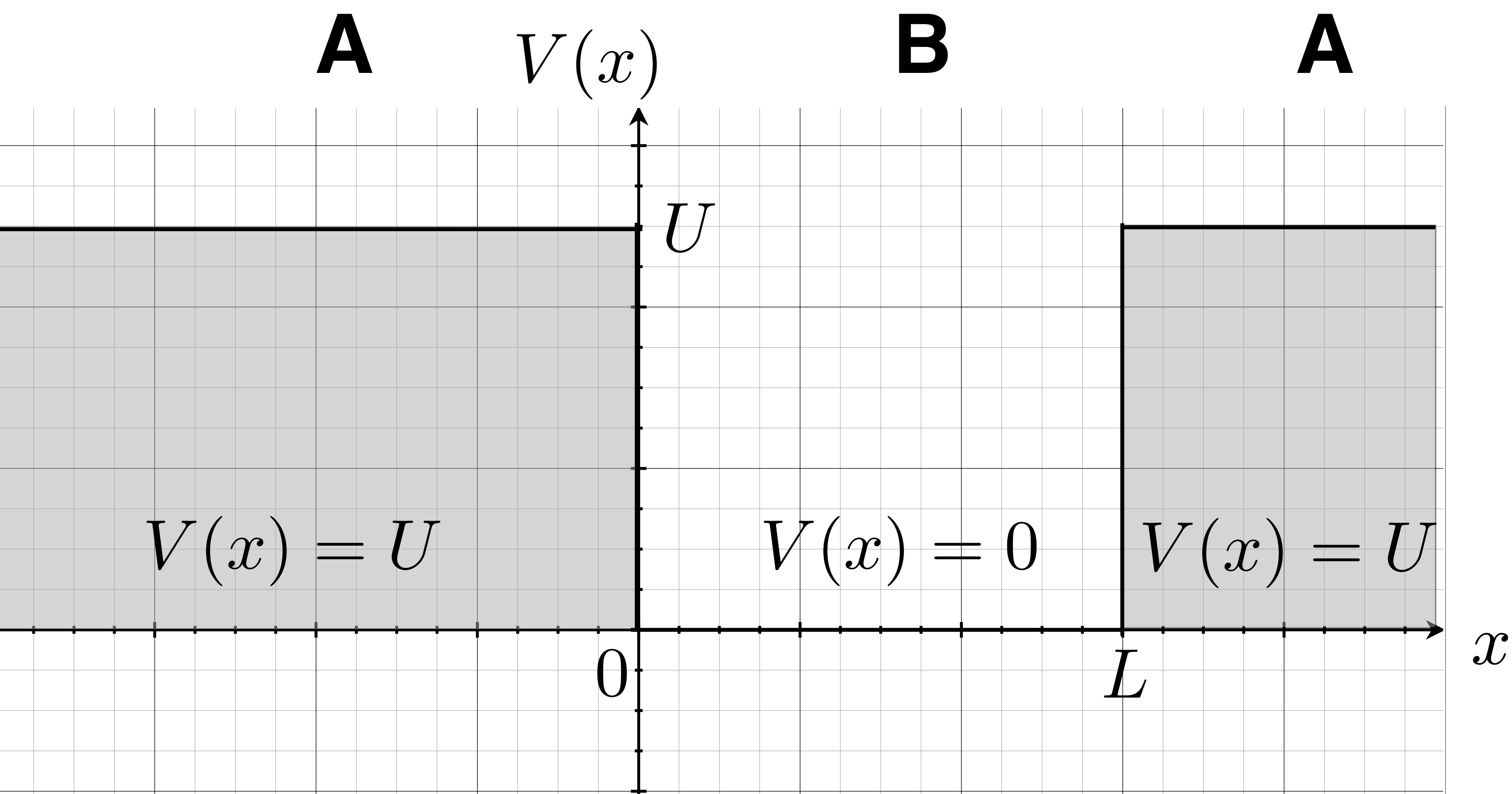
- To solve the **TISE**, we again split the problem up into **regions**, and then apply **boundary conditions**.
  - –**Region A)** where **V(x) = U.**
  - –**Region B)** where **V(x) = 0.**



Finite square well

– **Region B -** where **V(x) = 0.**
  - We have already solved the **TISE** for **V(x) = 0.**
  - Solutions:

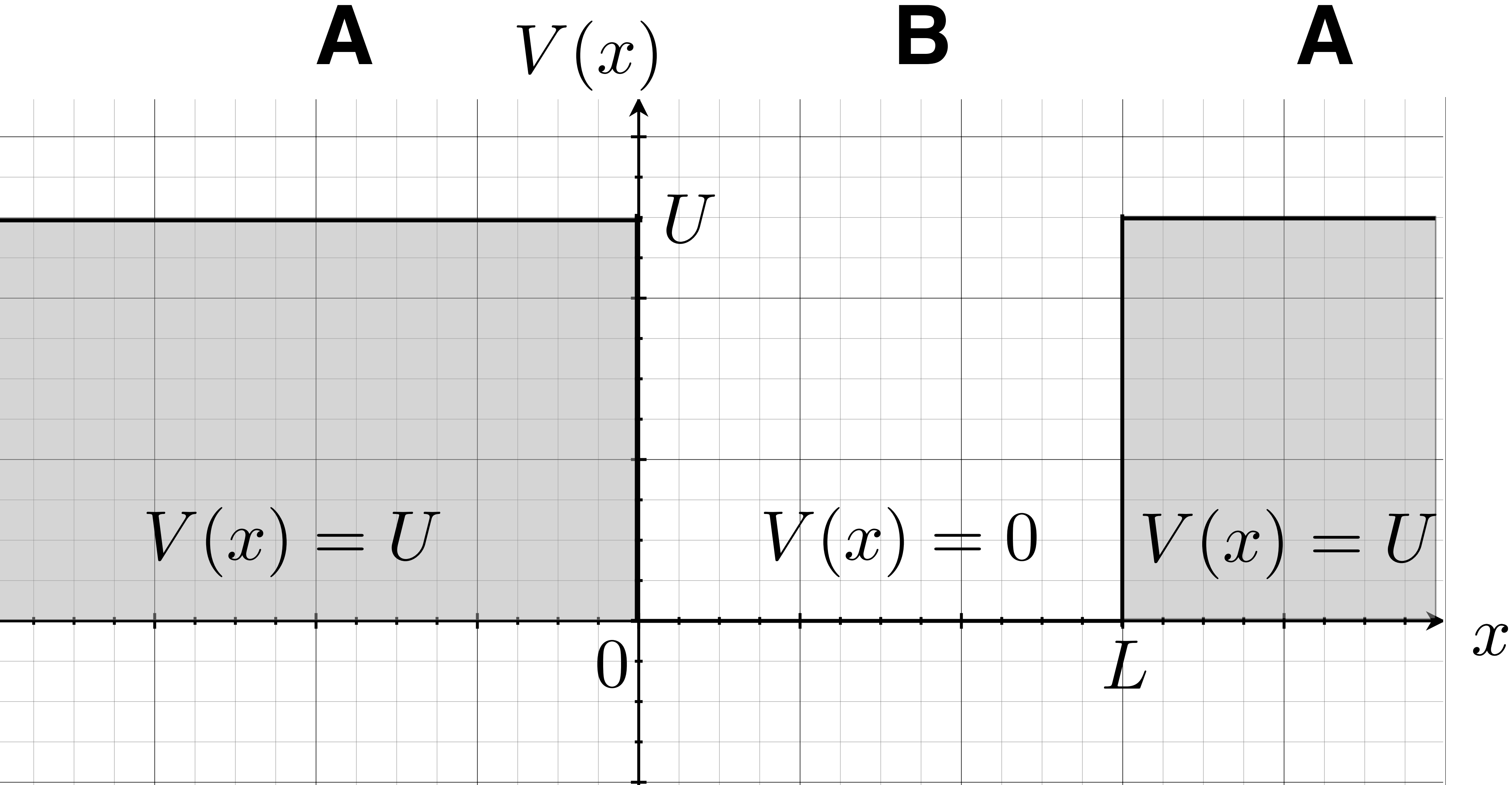
$$\psi_B(x) = a \sin\left(\frac{px}{\hbar} + c\right)$$



Finite square well

–**Region A -** where **V(x) = U.**

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U\psi(x) = E\psi(x)$$



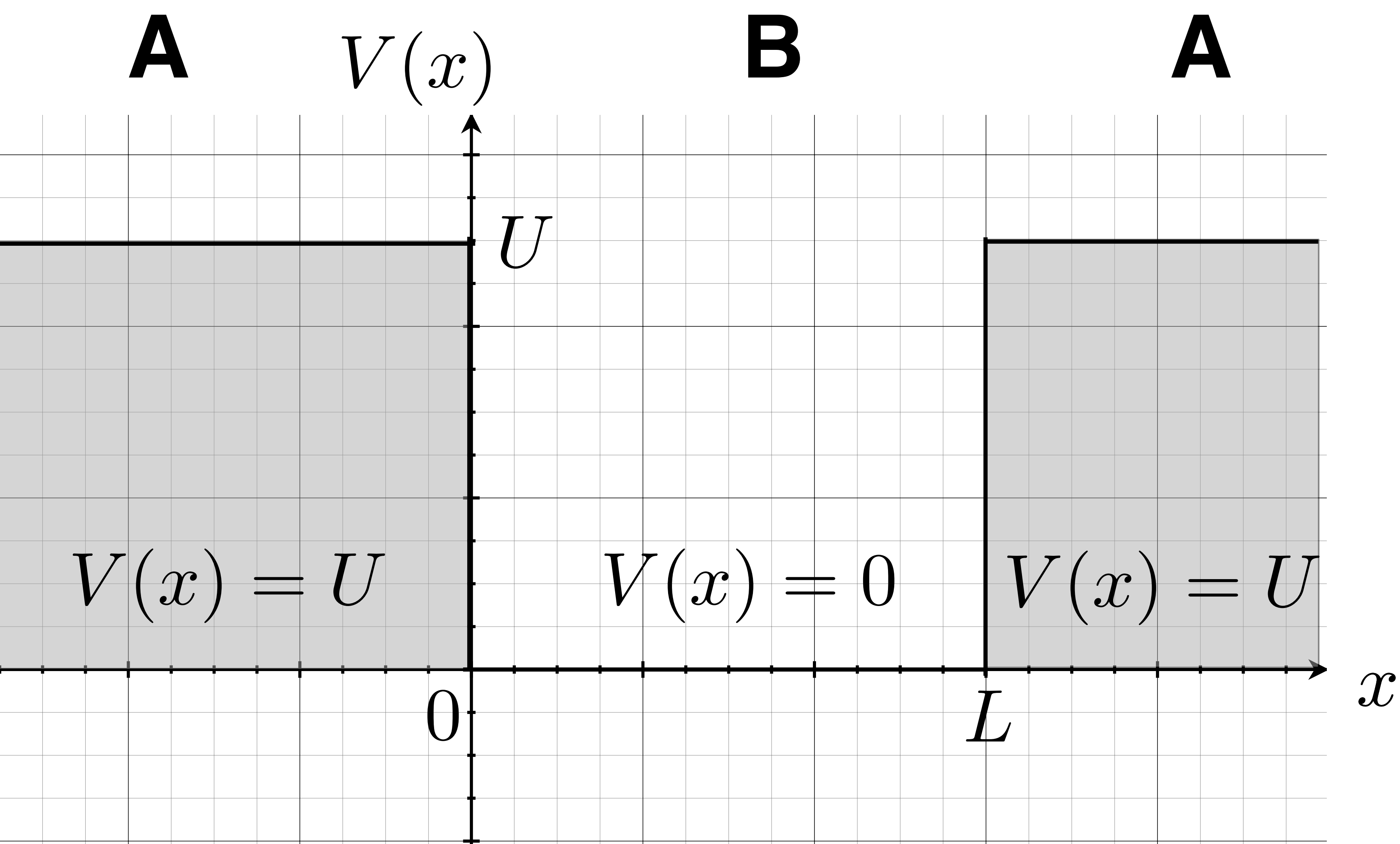
Hand-written Calculations

Finite square well

–When **E < U**, the solutions to the TISE have the form.

$$\psi_A(x) = Ae^{\pm Kx + C} \qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = a\sin\left(\frac{px}{\hbar} + c\right) \qquad 0 \leq x \leq L$$



$$K = \frac{\sqrt{|E-U|2m}}{\hbar}$$

$$p = \sqrt{E2m}$$

Finite square well

–When **E < U**, the solutions to the TISE have the form.

$$\psi_A(x) = Ae^{\pm Kx + C} \qquad x \leq 0 \;\; x \geq L$$

$$\psi_B(x) = a\sin\left(\frac{px}{\hbar} + c\right) \qquad 0 \leq x \leq L$$

–We can find the allowed values for ***A***, ***K***, ***C***, ***a***, ***p*** and ***c*** by imposing the boundary conditions:

- **ψ(x)** must be **continuous**
- **dψ(x)/dx** must be **continuous**
- **ψ(x)** must be **normalised**

$$K = \frac{\sqrt{|E-U|2m}}{\hbar}$$

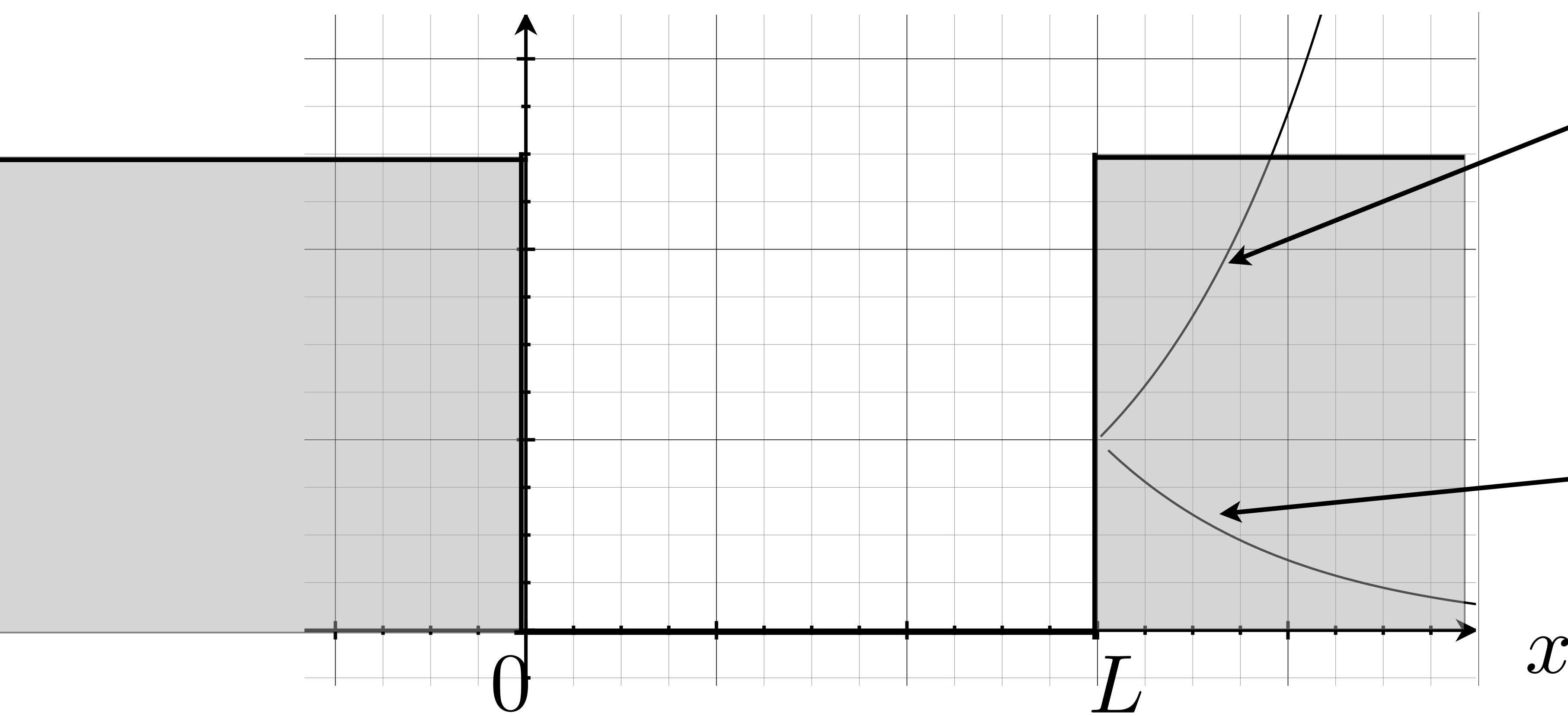
$$p = \sqrt{E2m}$$

Finite square well

- We will **not** perform the detailed calculation here (2nd year course) but let us see what this solution should look like.
- First, let's consider region A.

$$\psi_A(x) = Ae^{\pm Kx+C}$$

$$\psi_A(x) = Ae^{+Kx+C}$$

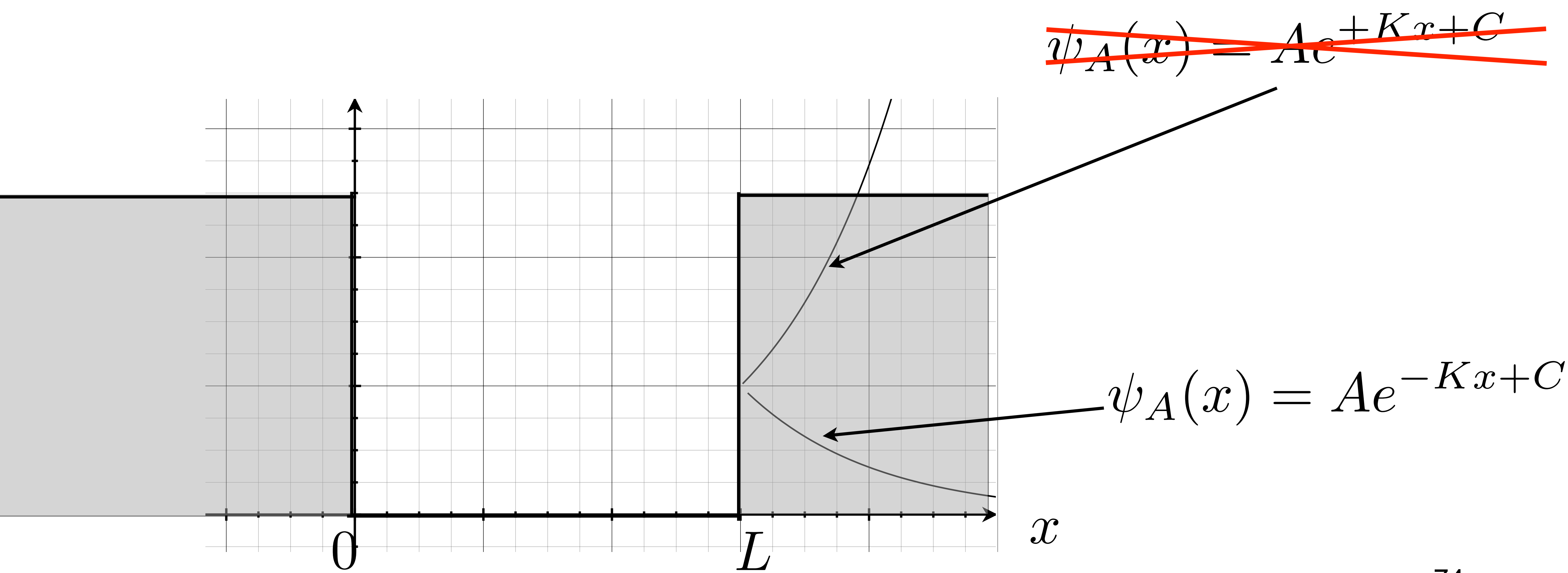


$$\psi_A(x) = Ae^{-Kx+C}$$

Finite square well

- One of these solutions **blows up** to infinity, as **x** tends to **infinity**.
- The **wavefunction** must **not** be infinite.
- Therefore in the region **x > L**, the wavefunction must be:

$$\psi_{x>L}(x) = Ae^{-Kx+C}$$

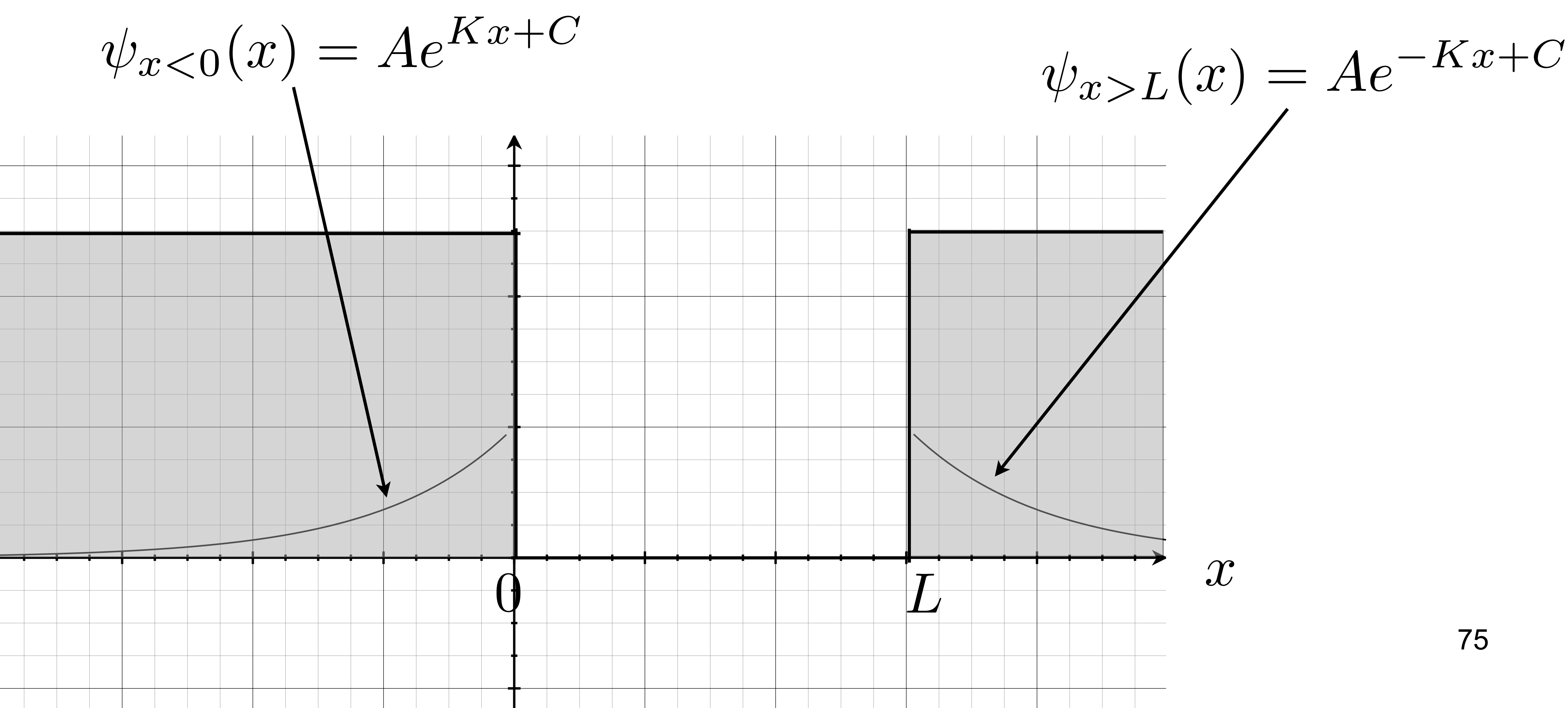


Finite square well

– Similarly, in the region, **x < 0** the wavefunction must be of the form:

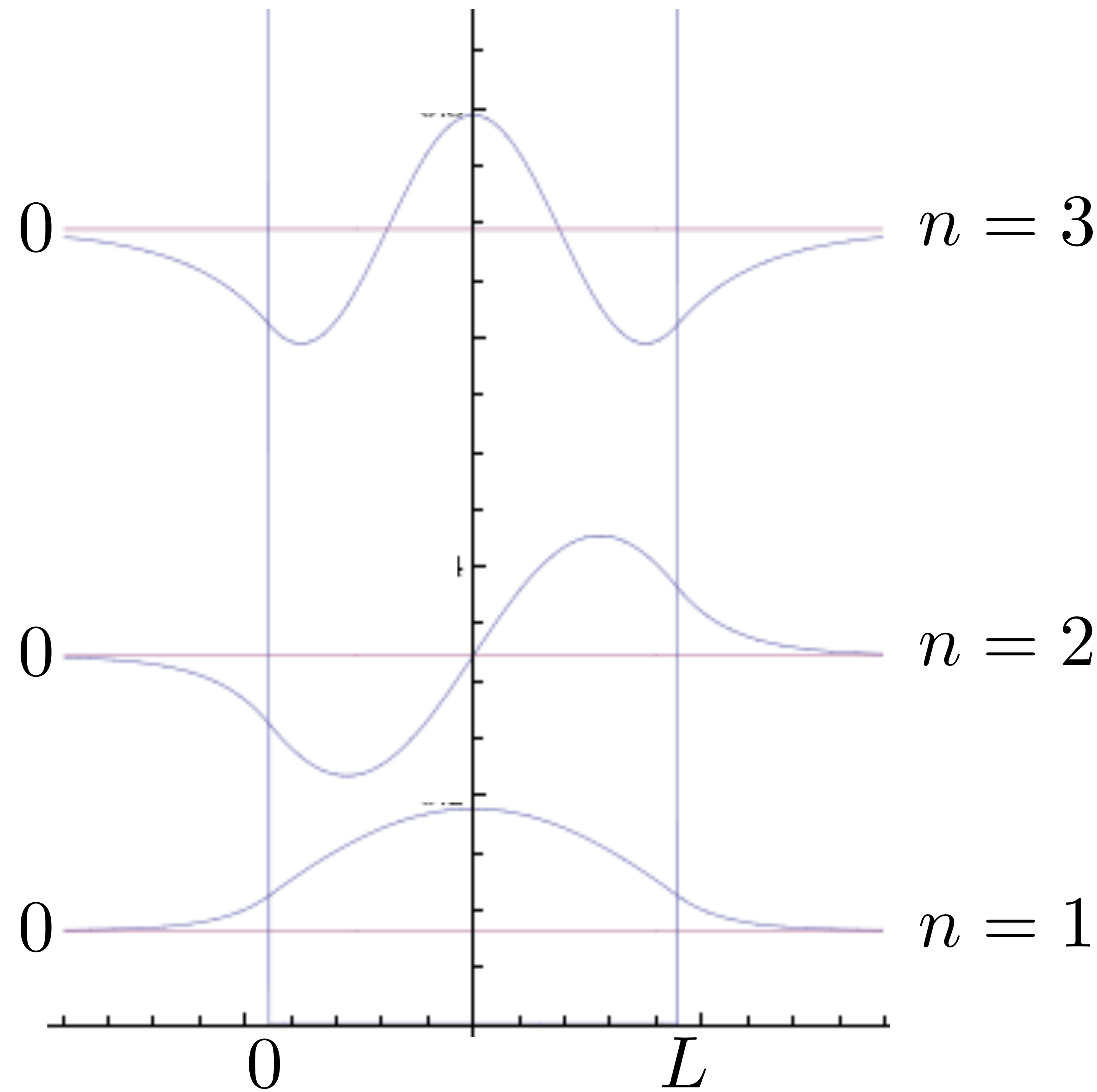
– NB A classical particle would **never** leave the well, but we see a **finite probability** of measuring the particle **outside the well**!

$$\psi_{x<0}(x) = Ae^{Kx+C}$$



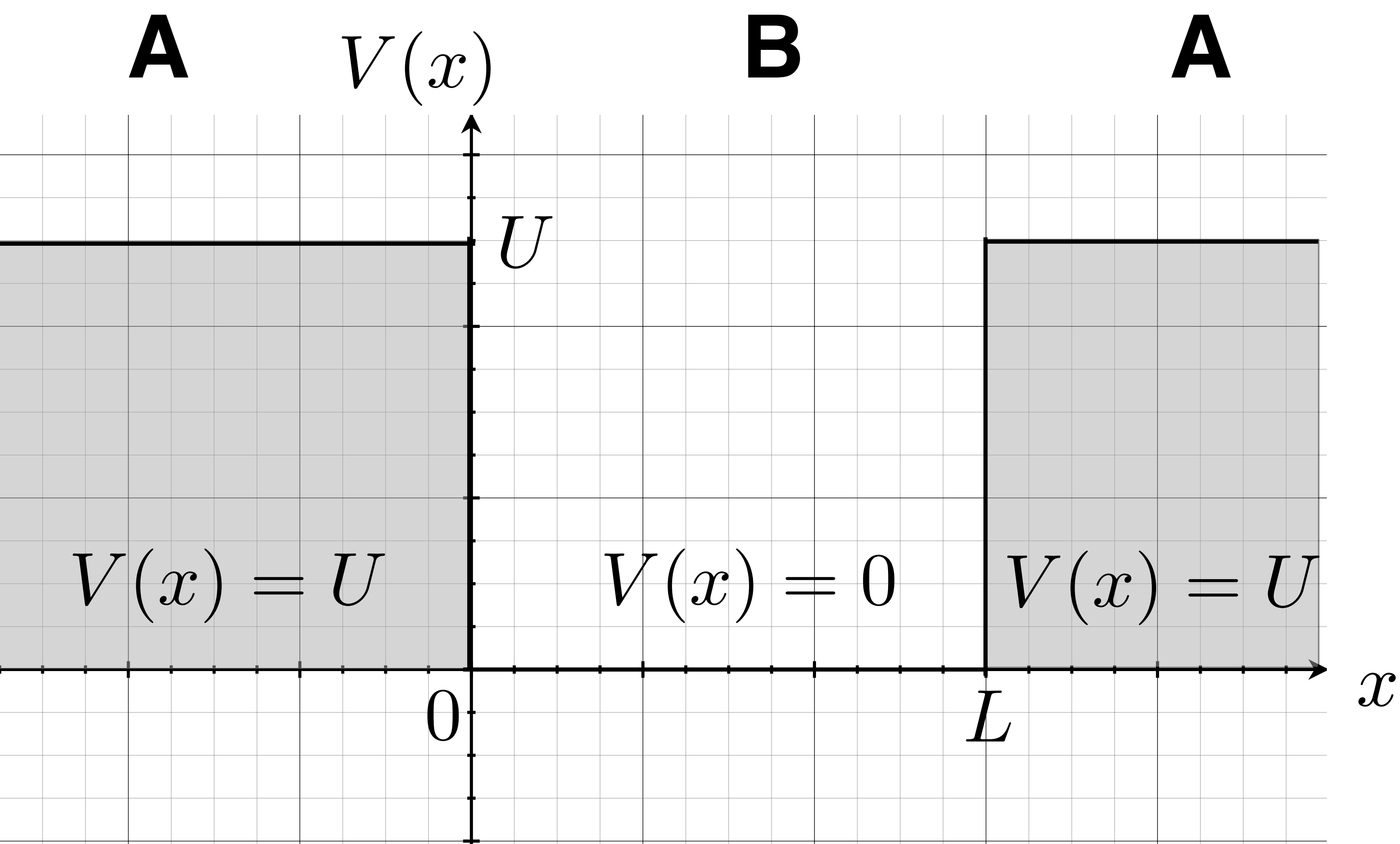
Finite square well

- Applying **boundary conditions** we can calculate the **wavefunctions** and allowed **energies**.
- The **energy** is still **quantised**.
- Wavefunction is :
  - **sinusoidal** inside well
  - **exponentially decaying** outside well
- All **wavefunctions** have a **non-zero** region **outside** the well.



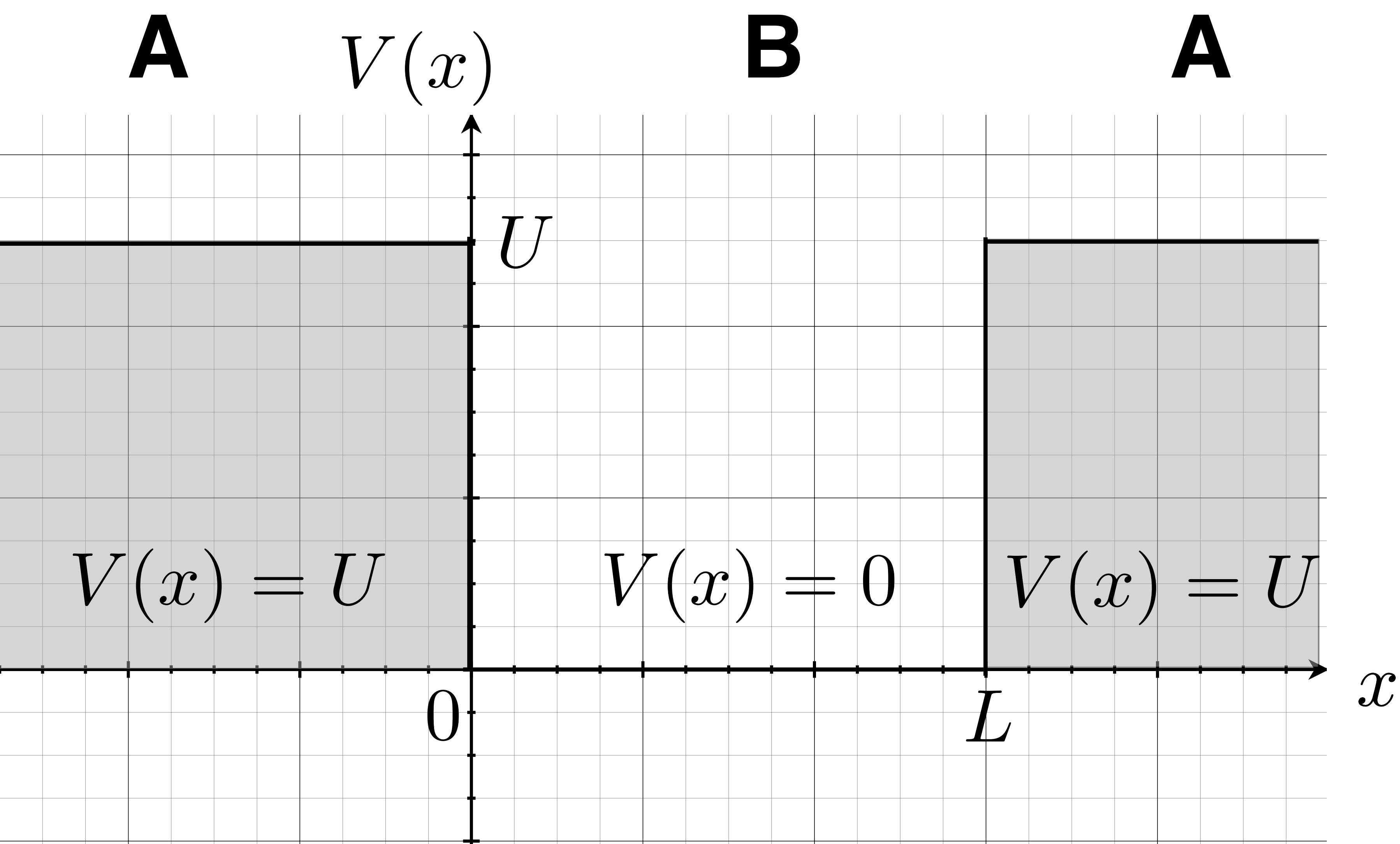
Finite square well

- So far we have assumed **E < U**, where a **classical particle** would **not** have **enough energy** to leave the well.
- We found the quantum particles have wavefunctions **mostly**, but **not entirely**, **inside** the well.
- We call these **bound states**.



Finite square well

- What happens when **E > U?**
- Where a **classical particle** would have **enough energy** to leave the well?



Hand-written Calculations

Finite square well

–When **E > U**, the solutions to the TISE have the form.

$$\psi_A(x) = a\sin\left(\frac{\tilde{p}x}{\hbar} + c\right) \qquad x \le 0 \;\; x \ge L$$

$$\psi_B(x) = a\sin\left(\frac{px}{\hbar} + c\right) \qquad 0 \le x \le L$$

–where $p = \sqrt{E2m}$ $\qquad \tilde{p} = \sqrt{(E-U)2m}$

–which we can rewrite:

$$E = \frac{p^2}{2m} \qquad E = \frac{\tilde{p}^2}{2m} + U$$

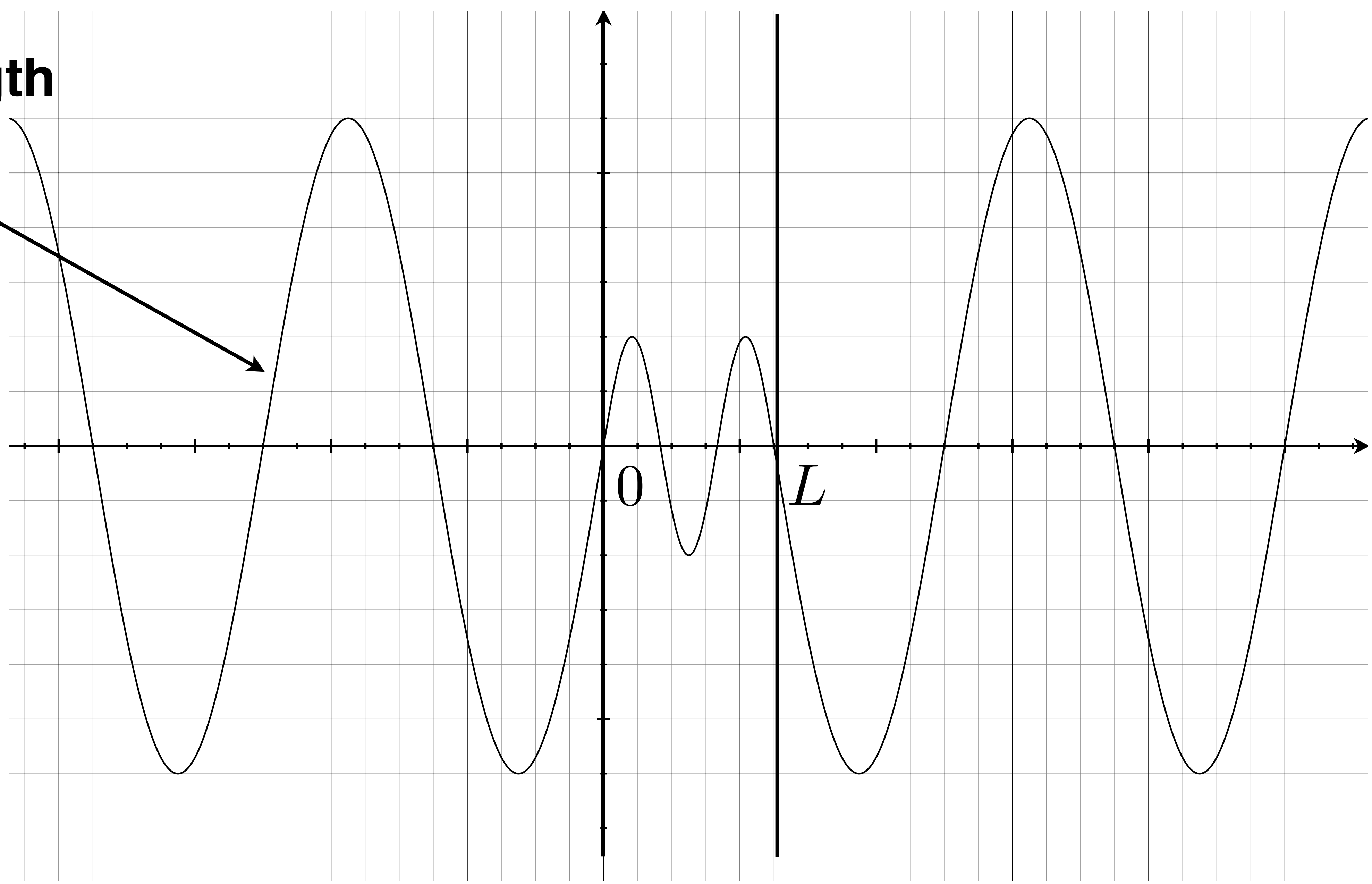
–These equations **match** the **energy equation** for a **classical particle**!

$$E_{\text{total}} = \frac{p^2}{2m} + V(x)$$

Finite square well

– Applying **boundary conditions**, we find **continuous sinusoidal** solutions:

Lower momentum = longer wavelength



- **We find solutions for all values of E > U, the energy in this case is not quantised.**

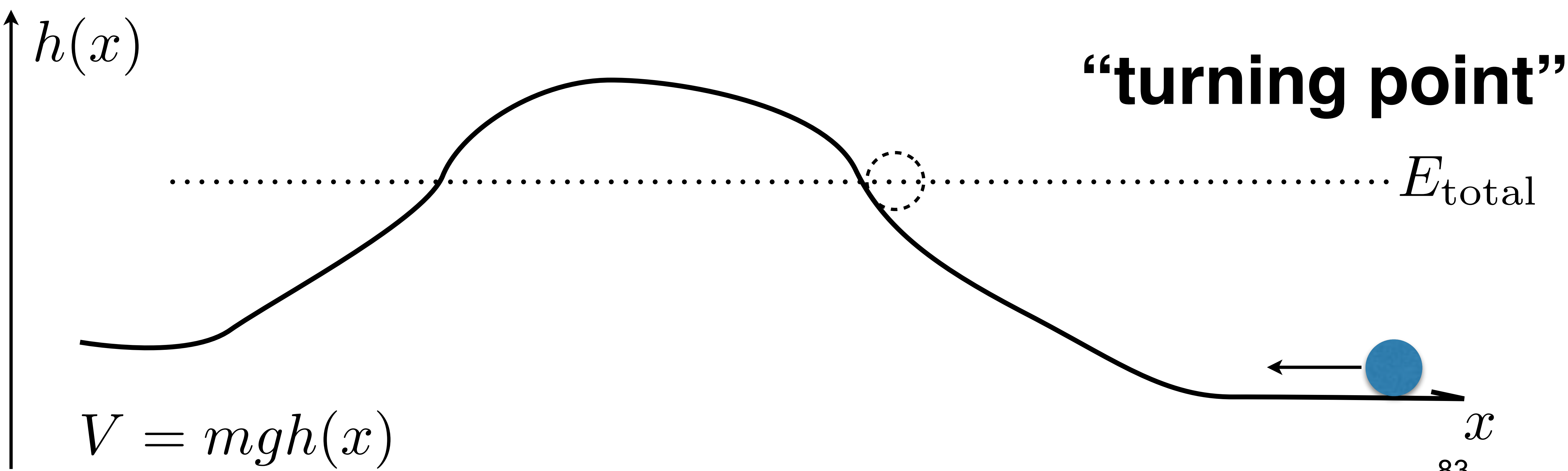
Finite square well - summary

- **Two** different types of behaviour:
  - **Bound states:** If **E < U** (classically particle trapped in well)
    - **Quantised** energies, **wavefunctions** largely (but not entirely) **localised** in well.
    - **Exponentially decay** outside well.
  - **Free states:** If E > U (classically particle not trapped)
    - Energy **not quantised**
    - Wavefunction **sinusoidal everywhere** (wavelength consistent with classical momentum).
- That the particle can be found **outside** the well, even if classically its **energy wouldn't allow it**, is a uniquely quantum behaviour, and related to the next topic - **quantum tunnelling**!

Quantum Tunnelling

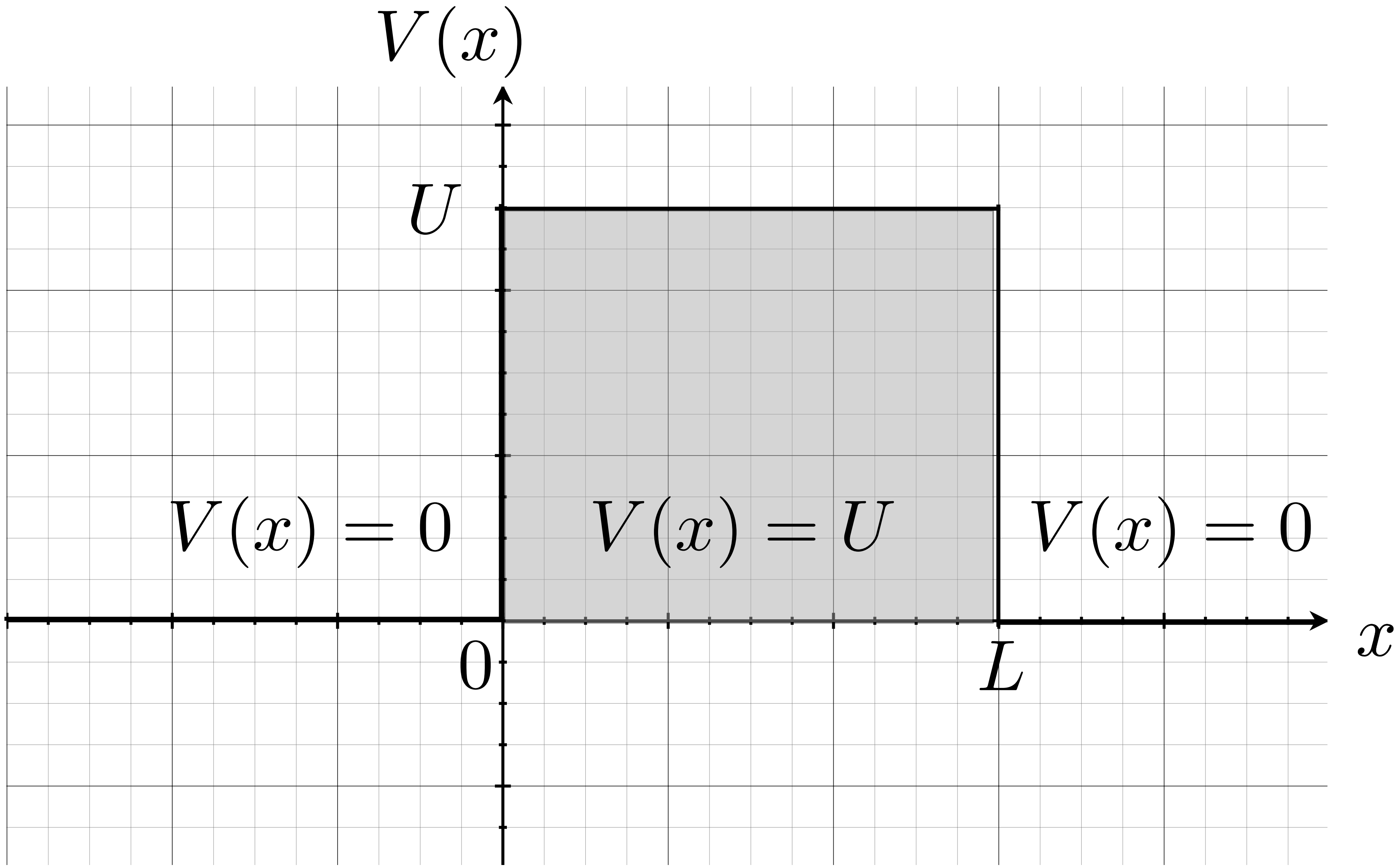
- In classical physics, potential energy can form a barrier.

$$E_{\text{total}} = \frac{p^2}{2m} + V(x)$$



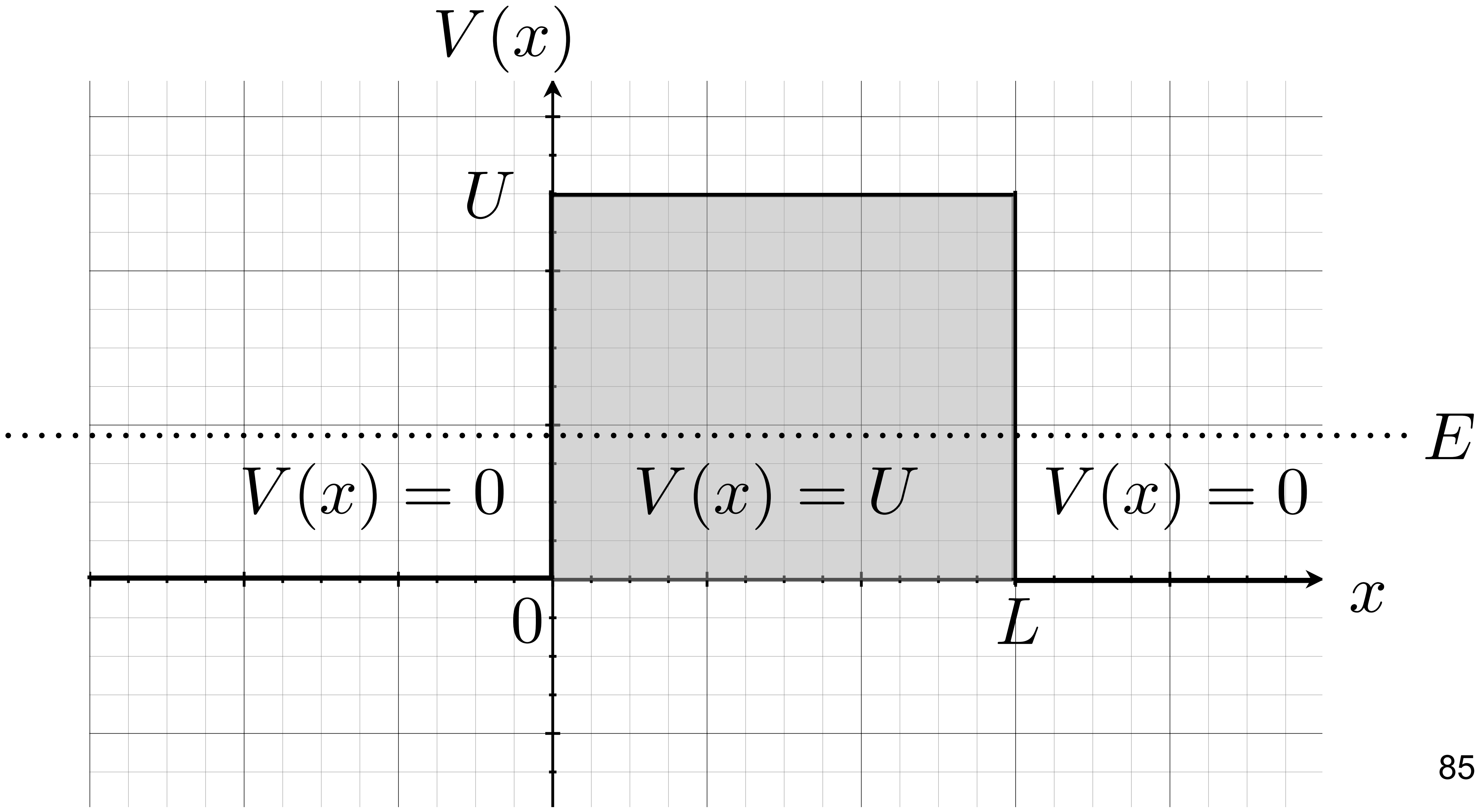
Quantum Tunnelling

- We can study a quantum potential barrier via the time-independent Schrödinger equation.



Quantum Tunnelling

- You will solve this in detail in future courses.
- However, the finite well gives us an insight.



Quantum Tunnelling

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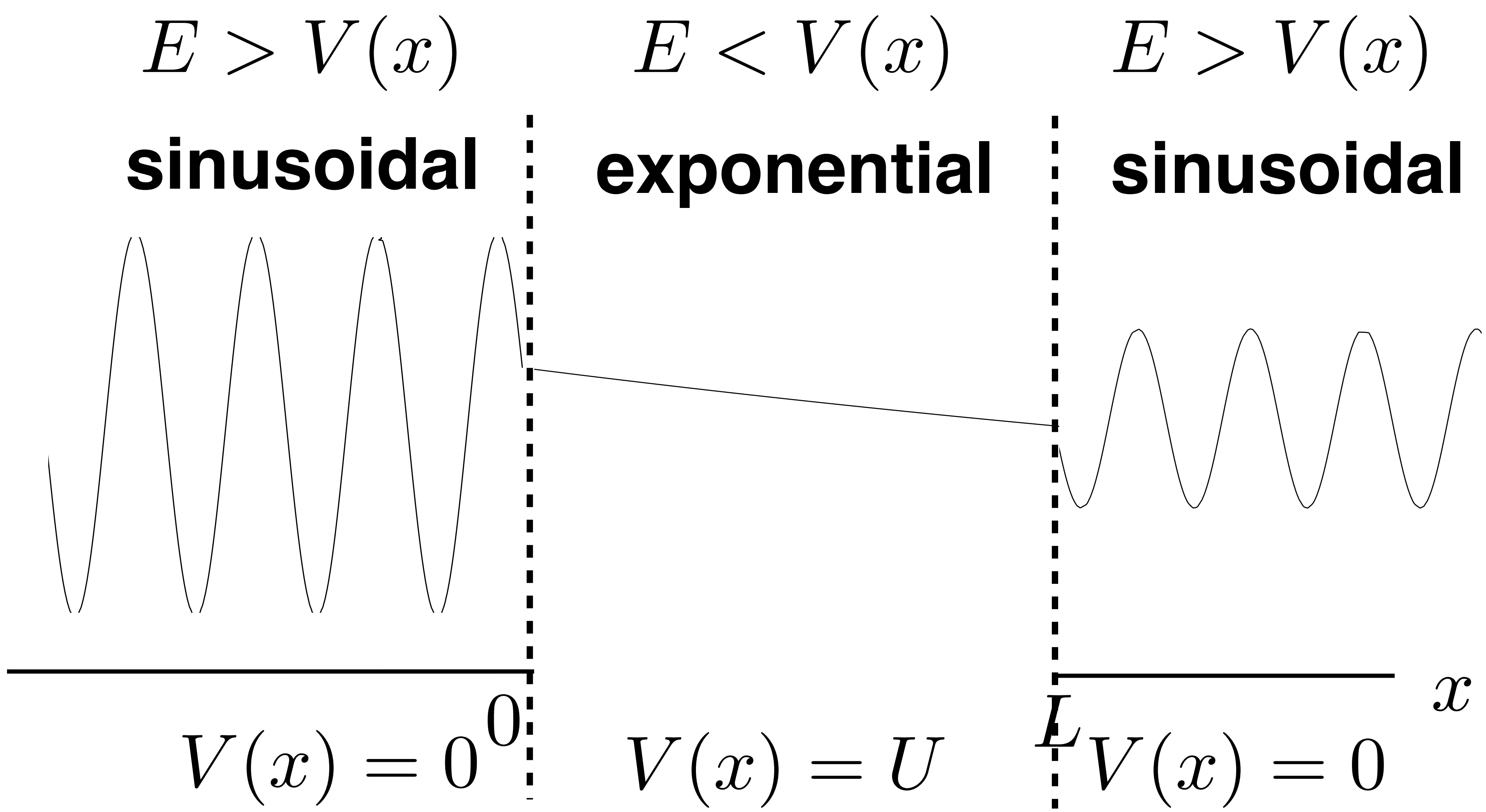
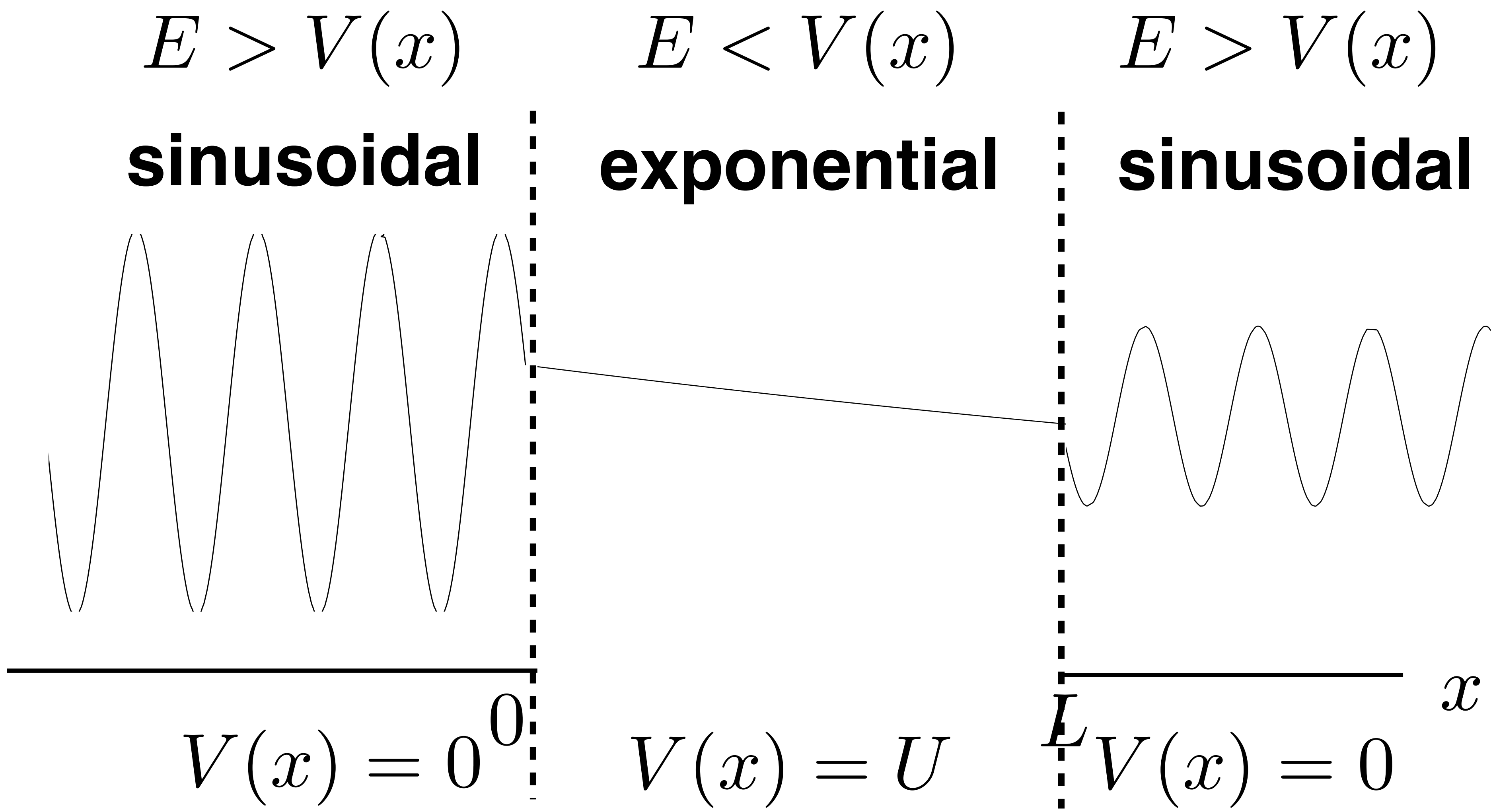


Quantum Tunnelling

- If a quantum particle (wavepacket) approaches the barrier, there is a finite probability that it will tunnel through.

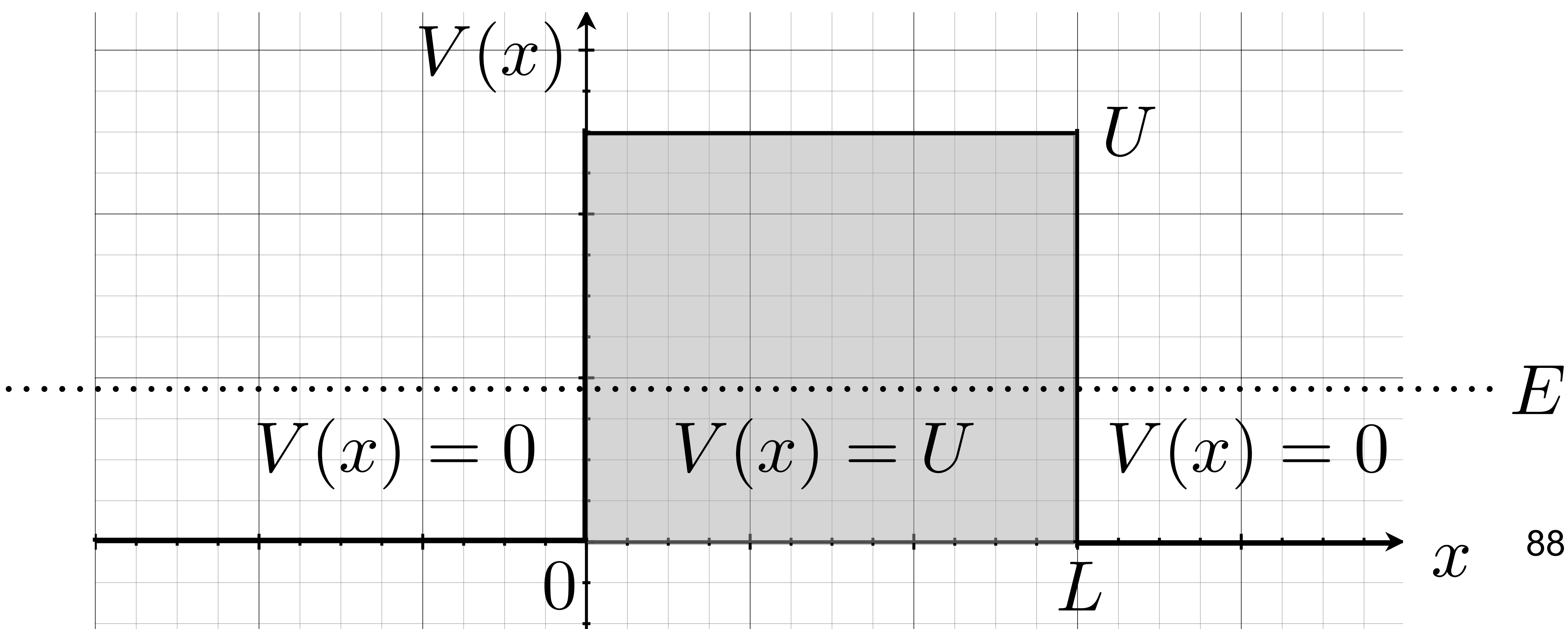


Quantum Tunnelling

- If a quantum particle (wavepacket) approaches the barrier, there is a finite probability that it will tunnel through.
- If the barrier is high (E<<U), the probability of tunnelling is given by:
- where

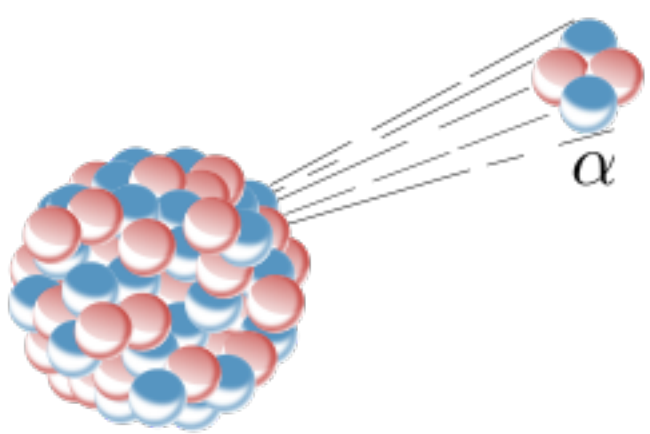
$$P = e^{-2CL}$$

$$C = \frac{\sqrt{2m(U-E)}}{\hbar}$$

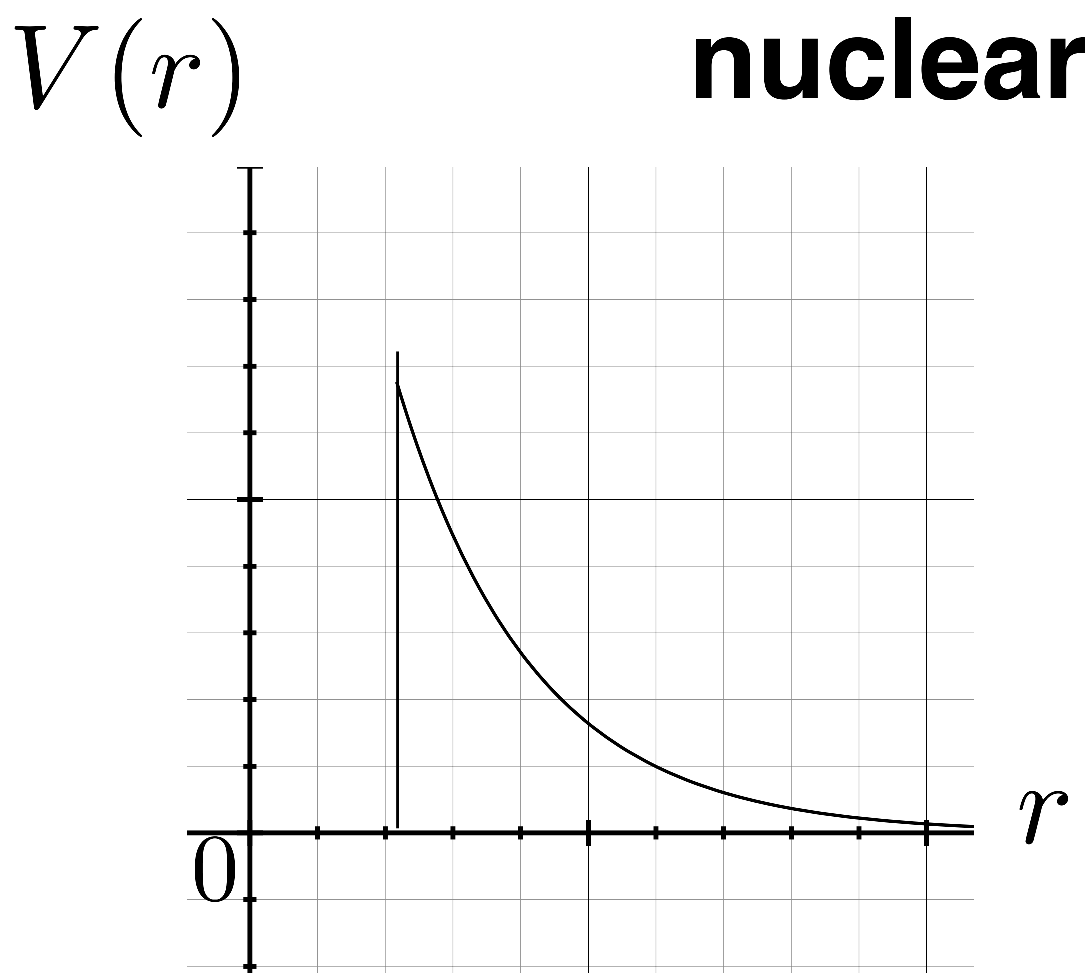


Quantum Tunnelling

- Quantum tunnelling is important in a number of physical processes.
- In radioactive decay (alpha decay), alpha particles tunnel through a potential barrier.
- This gives rise to the probabilistic nature of radioactive decay.



nuclear potential

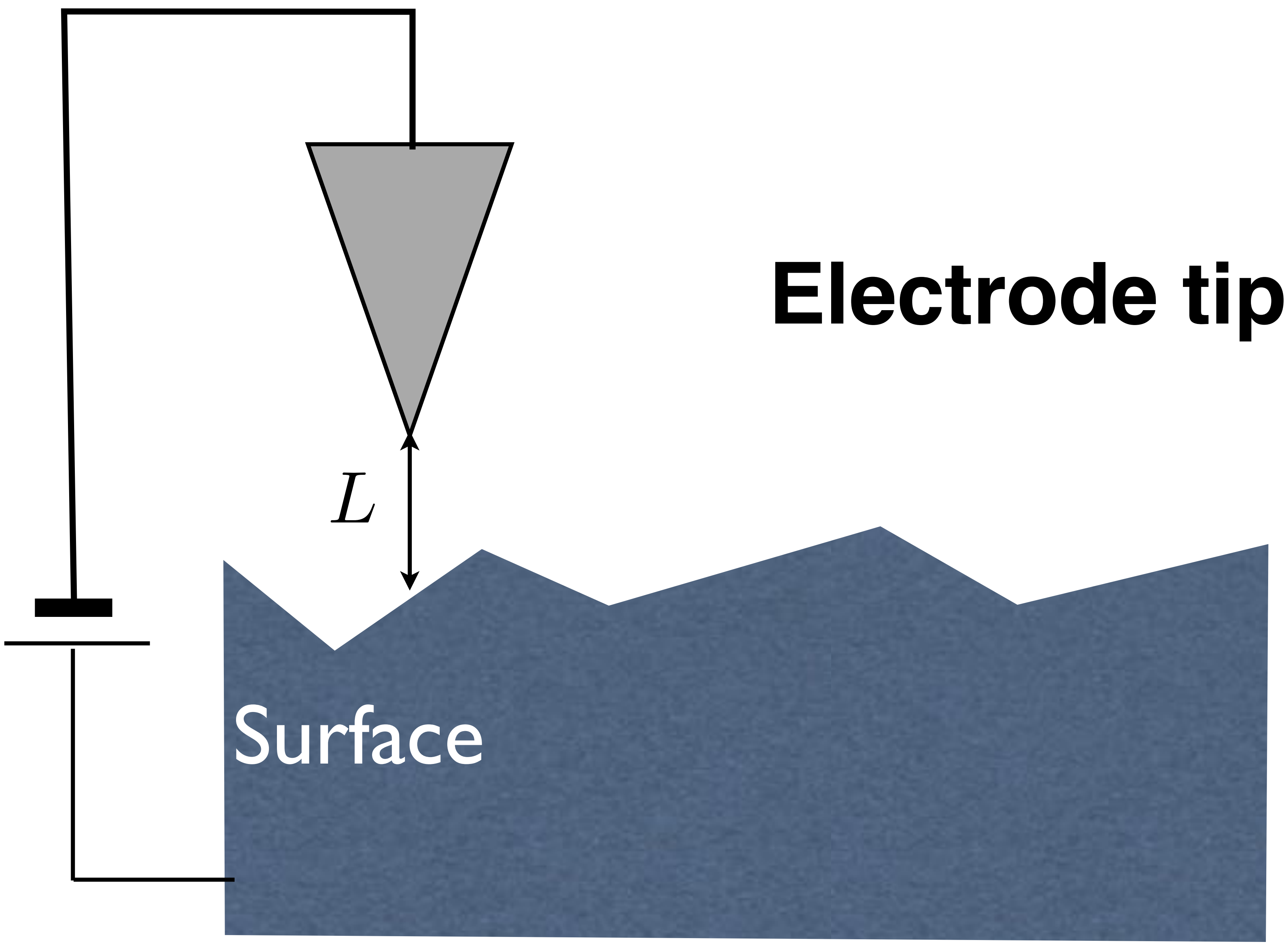


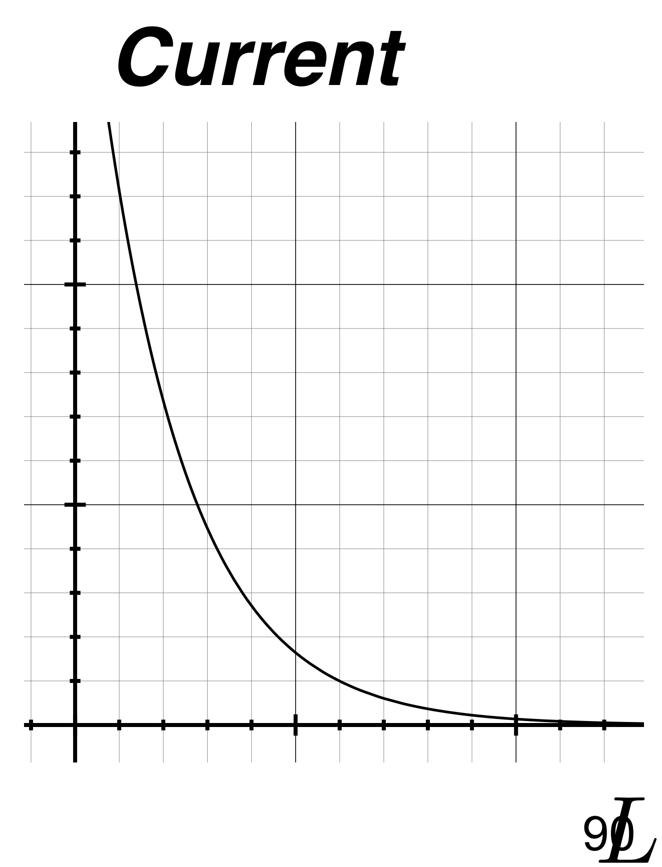
Quantum Tunnelling

- A scanning tunnelling microscope is one of our most precise tools for measuring surfaces.

- The rate of current is proportional to tunnelling probability.

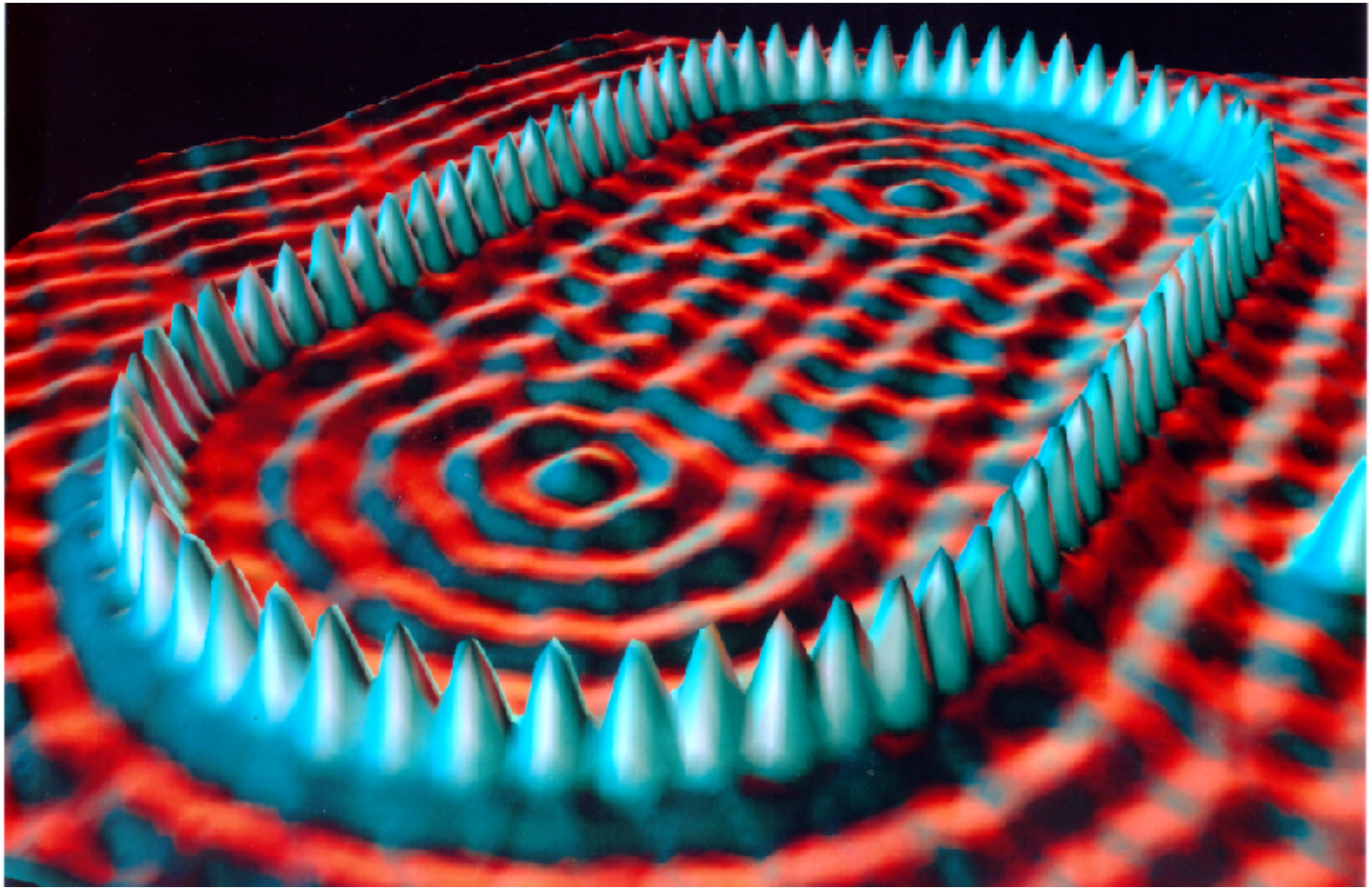
$$P = e^{-2CL}$$





Quantum Tunnelling

- This is a STM image taken by IBM.
- Individual atomic sites, and wave-behaviour can be resolved!



Part 5: Summary so far…

- We introduced the Time-independent Schrödinger Equation, which connects **energies** and **wave-functions**.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

- And saw how to **solve it** to study the physics of **potential wells** (infinite and finite).
- We also used it to study **quantum tunnelling** and its applications.
- Next week, we apply these tools to develop a **quantum model** of the **atom**.