Phys 231 2021

Lecture 23

Tues: HW by 5pm

Weds: Read 5.6, 5.7

Infinite well

The particle in an infinite well represents the first example of a situation where we can follow a general scheme:

Schrödinger eqn

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$$

→ TISE

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

→ Energy eigenstates + energies

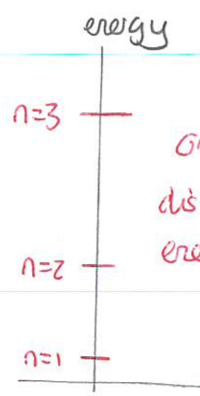
Specifically for a particle in a well from $0 \leq x \leq L$ we found that

The energy eigenstates are labeled by $n = 1, 2, 3, \ldots$ and are

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

with energy

$$E_n = n^2\frac{\hbar^2\pi^2}{2mL^2}$$



only certain discrete energies

This is also the first example where we find discrete energies and hence a discrete emission or absorption spectrum.

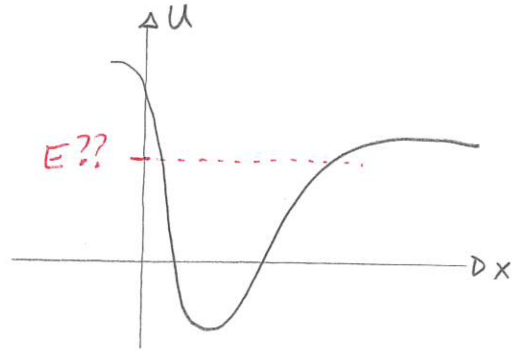
Quiz 1

Bound particles: classical

The presence of discrete energy levels is typical of situations where particles are bound. This means that their motion is restricted to a finite region of space. We consider classical and quantum descriptions of such particles. These will both use a constraining potential.

In classical physics the total energy of a particle is

$$E = K + U(x)$$



Then $K \geq 0$ implies that we must have

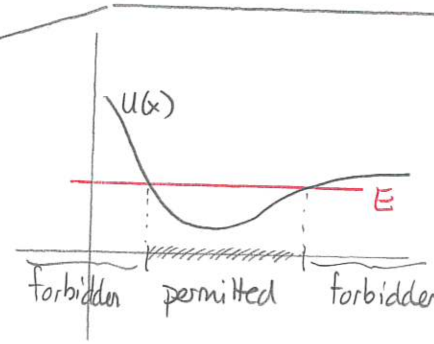
$$U(x) \leq E$$

If there is a portion of $U(x)$ which is concave up then this can result in possible constraints on a particle location.

Quiz2 100%

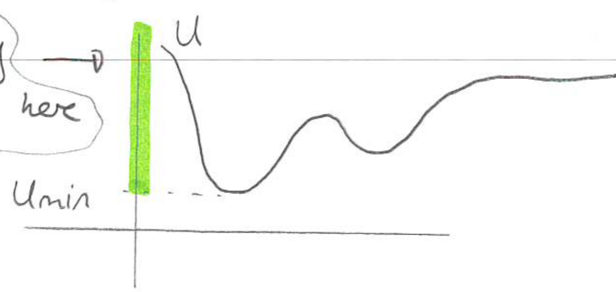
We see that

> In classical physics given energy E the particle is restricted to locations x such that $U(x) \leq E$. Any location where $U(x) > E$ is not possible for the particle and is forbidden



This itself does not say what the classical energy is. However it does constrain the classical energy to be above the minimum potential energy.

total energy E anywhere here



Total energy is continuous

Bound particles: quantum

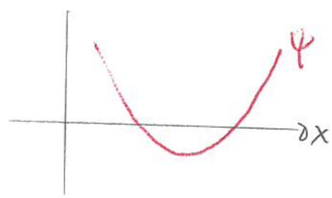
Consider a similar situation in quantum theory. We seek a wavefunction $\psi(x)$ that corresponds to a particular energy E. Then the TISE requires

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

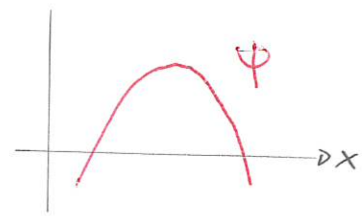
$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left[E - U(x)\right]\psi$$

For real wavefunctions, the sign of the second derivative describes the concavity of the function. Specifically:

$\frac{d^2\psi}{dx^2} > 0 \Rightarrow$ concave up



$\frac{d^2\psi}{dx^2} < 0 \Rightarrow$ concave down



We see that roughly

concavity = [negative constant] × [total energy larger/smaller than U] × [sign wavefunction]

There are two cases:

1) Classically permitted region $(E > U(x))$

$$\frac{d^2\psi}{dx^2} = \underset{\text{number}}{\text{negative}} \times \psi$$

In this case the wavefunction "attempts to return to the x axis"

Quiz 3 20% – 70%

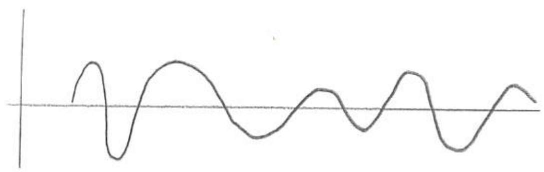
Here if $\psi > 0$ we have $\frac{d^2\psi}{dx^2} < 0 \Rightarrow$ concave down

$\psi < 0$ " " $\frac{d^2\psi}{dx^2} > 0 \Rightarrow$ " "

This generally produces oscillatory wave functions

$E > U$

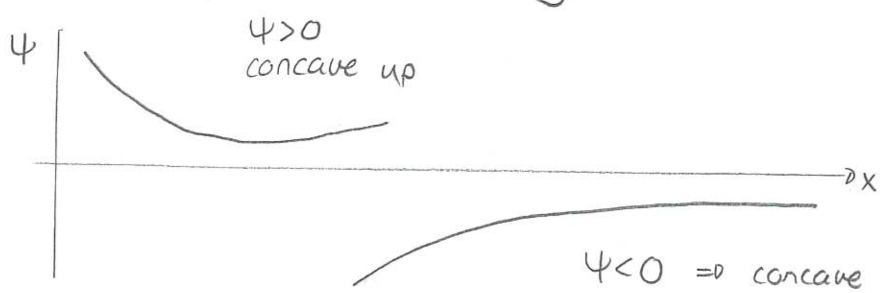
classically permitted



2) Classically forbidden region $(E < U(x))$

$$\frac{d^2\psi}{dx^2} = \text{positive number} \times \psi$$

This does not produce oscillatory functions



Immediately this shows:

In quantum theory the wavefunction can be non-zero in regions which are classically forbidden $(E<U)$. This means that there can be a non-zero probability of locating the particle in a classically forbidden region.

The exact nature of such solutions depends on the potential but there are two constraints:

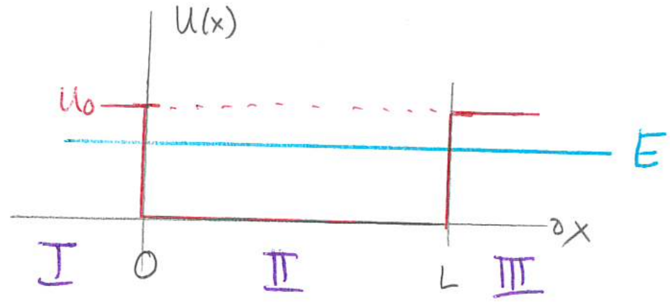
1) the wavefunctions and their derivatives must match at the junctions between regions.

2) the wavefunction must be normalized.

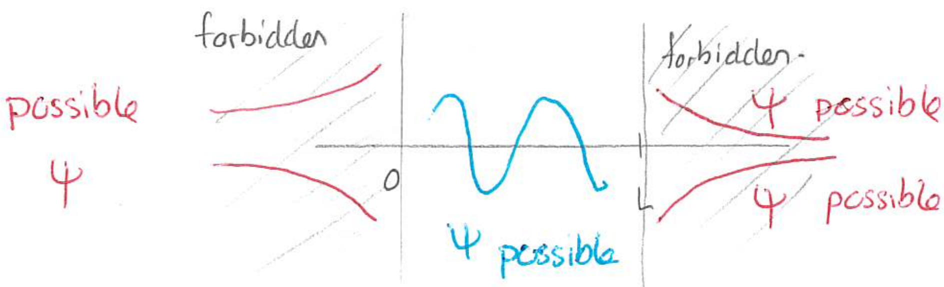
Finite well

In the finite well

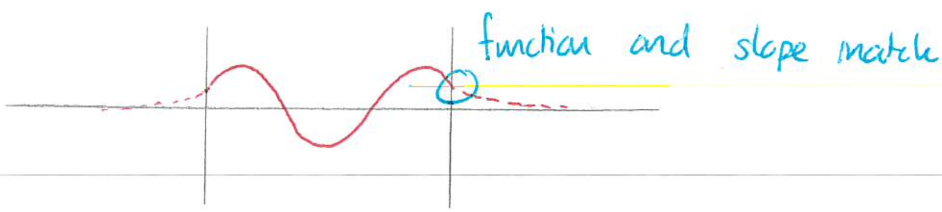
$$U(x) = \begin{cases} 0 & 0 < x < L \\ U_0 > 0 & \text{otherwise.} \end{cases}$$



We consider possible energies $E < U_0$. We can consider solutions in each region. First consider either of the classically forbidden regions. The solution must be concave away from the axis and must → 0 at infinite distances for the wavefunction to converge



Then in the permitted region the solution will be concave toward the axis and oscillate. These must match at the boundary



We will see that these constrain the possible energies and solutions.