7 Particles in one-dimensional potentials

7.1 Infinite potential well

Energy diagram

(taken from McIntyre, Quantum Mechanics)

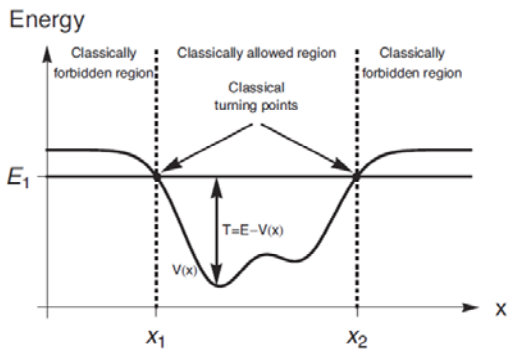


Figure 5.8 A generic potential energy well.

infinite potential well

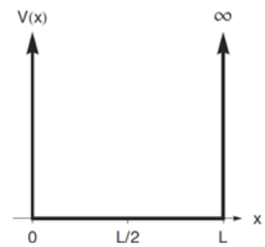


Figure 5.9 Infinite square potential energy well.

Hamilton Operator:

$$\hat{H} = \frac{1}{2m}\hat{P}^2 + V(\hat{X})$$

measurements of energy

➔ projection onto energy eigenstates!
(associated with energy eigenvalues)

Potential

$$V(x) = \begin{cases} \infty & -\infty < x < 0 \\ 0 & 0 \le x \le L \\ \infty & L < x < +\infty \end{cases}$$

It turns out that (in contrast to classical mechanics) we can find only an infinite (but discrete) set of of energies in the system!

Solving Strategies: particle in potential

$$\boxed{\frac{d}{d\,t}|\Psi(t)\rangle = -\frac{i}{\hbar}H|\Psi(t)\rangle}$$

Initial state: $|\Psi(0)\rangle$ mass: m

1) Find Eigensystem of H:

$$\hat{H} = \frac{\hat{P}_x^2}{2m} + V(\hat{X})$$

$$\boxed{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi_E(x) = E\;\Psi_E(x)}$$

2) Decompose initial state into eigenstates of H

$$|\Psi(0)\rangle = \sum_n \langle E_n|\Psi(0)\rangle\;|E_n\rangle$$

$$\boxed{\langle E_n|\Psi(0)\rangle = \int\; dx\;\Psi^*_{E_n}(x)\;\Psi(x,0)}$$

3) Write down final solution

$$|\Psi(t)\rangle = \sum_n \langle E_n|\Psi(0)\rangle\; e^{-i\frac{E_n t}{\hbar}}\;|E_n\rangle$$

$$\boxed{\Psi(x,t) = \sum_n \langle E_n|\Psi(0)\rangle\; e^{-i\frac{E_n t}{\hbar}}\;\Psi_{E_n}(x)}$$

7.1.1 Eigensystem of H (Eigenvalue E, eigenstate $\psi_E(x)$): eigenfunction form in each section

Section I and III:

$\psi_E(x) = 0$ for physical reasons (infinite potential)

$$\left[-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2} + \infty\right]\psi_E(x) = E\,\psi_E(x)$$

infinite finite

Section II:

General solution:
(assume E>0)

$$\psi_E(x) = A' e^{i\frac{p}{\hbar}x} + B' e^{-i\frac{p}{\hbar}x}$$

(momentum eigenstates restricted to section II)

$$\Rightarrow \psi_E(x) = \begin{cases} 0 & \mathrm{I}, \mathrm{III} \\ A' e^{i\frac{p}{\hbar}x} + B' e^{-i\frac{p}{\hbar}x} & \mathrm{II} \end{cases}$$

is a *candidate* for an eigenfunction of the Hamiltonian corresponding to the infinite well!

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

7.1.2 Matching conditions at interface

Wave functions are continuous!

mathematical condition, solution has to solve Schrödinger equation on the whole line!
we will have to expand more on this in the next section ...

Reformulation of general solution

$$\psi_E(x) = \begin{cases} 0 \\ A\cos\left(\frac{px}{\hbar}\right) + B\sin\left(\frac{px}{\hbar}\right) \end{cases}$$

Boundary conditions:

i) $\psi_E(0) = 0$ ii) $\psi_E(L) = 0$

i) $\Rightarrow A = 0$

ii) $\Rightarrow p\frac{L}{\hbar} = n\pi \qquad n = 1, 2, 3, \ldots$

Solutions possible only for a discrete set of values of momentum p!
And with that, only for discrete values of energy E!

$$E = \frac{p^2}{2m} \qquad p = \frac{n\pi\hbar}{L}$$

$$\Rightarrow E = \frac{\pi^2\hbar^2}{2L^2 m} n^2$$

Note that n=0 is not a valid eigenenergy, as then the wave function would vanish!

7.1.3 Normalization Condition

$$\psi_E(x) = \begin{cases} 0 & \mathrm{I}, \mathrm{III} \\ B \sin \frac{\sqrt{2mE_n}\, x}{\hbar} & \mathrm{II} \end{cases}$$

$$\Rightarrow \int_{-\infty}^{+\infty} dx\, |\psi_E(x)|^2 = \int_0^L |B|^2 \sin^2 \frac{\sqrt{2mE_n}\, x}{\hbar}$$

$$= \ldots = |B|^2 \frac{L}{2}$$

$$\Rightarrow B = \sqrt{\frac{2}{L}}$$

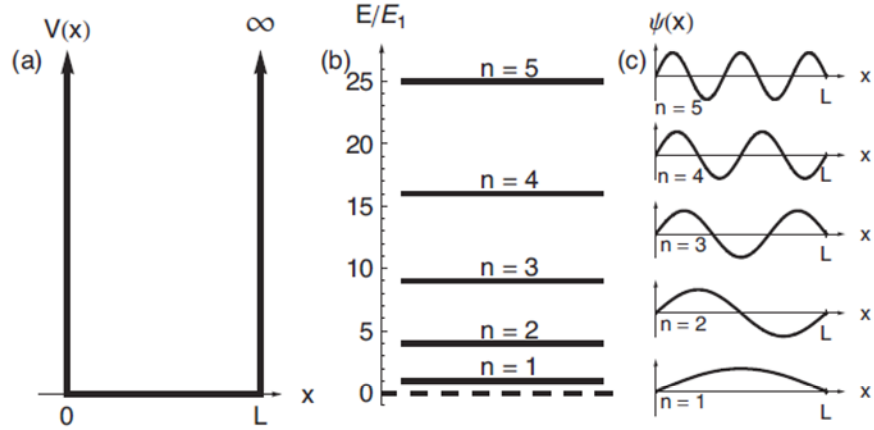
$$\boxed{\Rightarrow \psi_{E_n}(x) = \begin{cases} 0 & \mathrm{I}, \mathrm{III} \\ \sqrt{\frac{2}{L}} \sin \frac{\sqrt{2mE_n}\, x}{\hbar} & \mathrm{II} \end{cases} \qquad E_n = \frac{\pi^2\hbar^2}{2L^2 m} n^2 \qquad n = 1, 2, 3, \ldots}$$

These are now the complete set of eigenstates and eigenvalues of our Hamilton Operator!

7.1.4: Eigensystem of H: Results

Infinite Potential Well: Results

(taken from McIntyre, Quantum Mechanics)



Sharp energy values for energy eigenstates only

- discrete energy spectrum

$$E_n = \frac{\pi^2\hbar^2}{2L^2m}n^2 \qquad \text{n = 1,2,3 ...} \qquad \Psi_{E_n}(x) = \begin{cases} 0 & \mathit{outside} \\ \sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L} & \mathit{inside} \end{cases}$$

- Ground state with energy $E_1 > 0$

Reminder: Orthogonality of Eigenstates

The eigenstates for different Energy states are orthogonal:

$$\int_{-\infty}^{+\infty} dx\, \psi^*_{E_n}(x)\, \psi_{E_m}(x) = \int_0^a dx\, \psi^*_{E_n}(x)\, \psi_{E_m}(x)$$

$$= \delta_{n,m} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$$

(Kronecker Delta)

Reminder: Completeness relation

For the interval 0<x<a the eigenfunctions ψ_{E_n} form an orthonormal basis

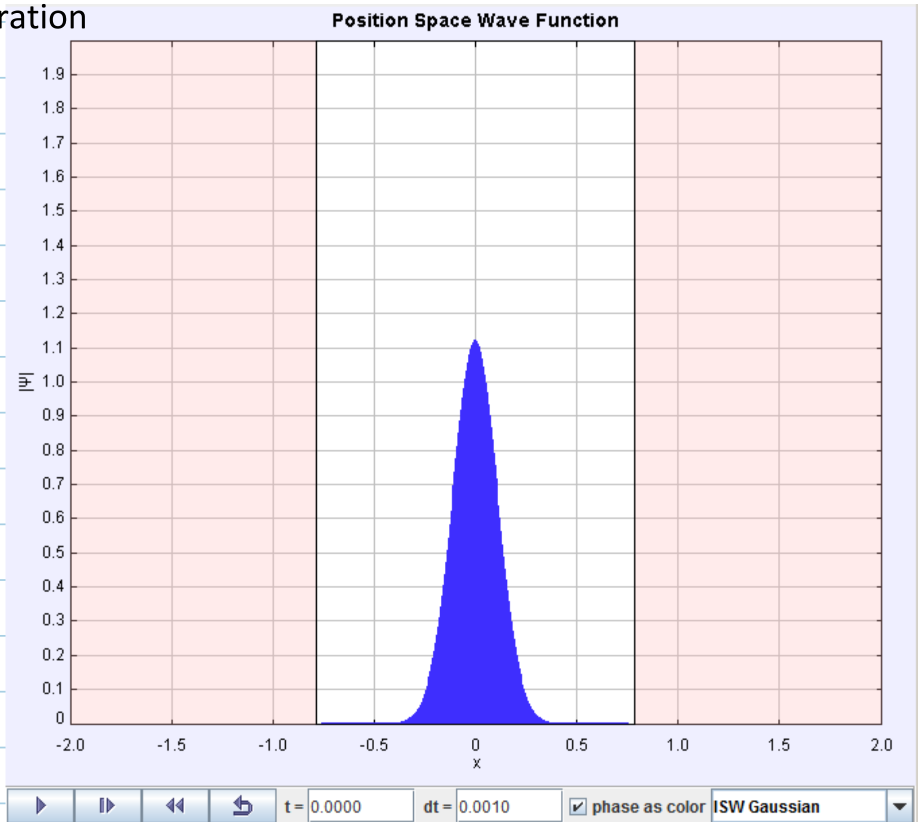
Any square integrable function f(x) with zeros's at the boundary can be expanded as

$$f(x) = \sum_{n=1}^{\infty} c_n\, \psi_{E_n}(x)$$

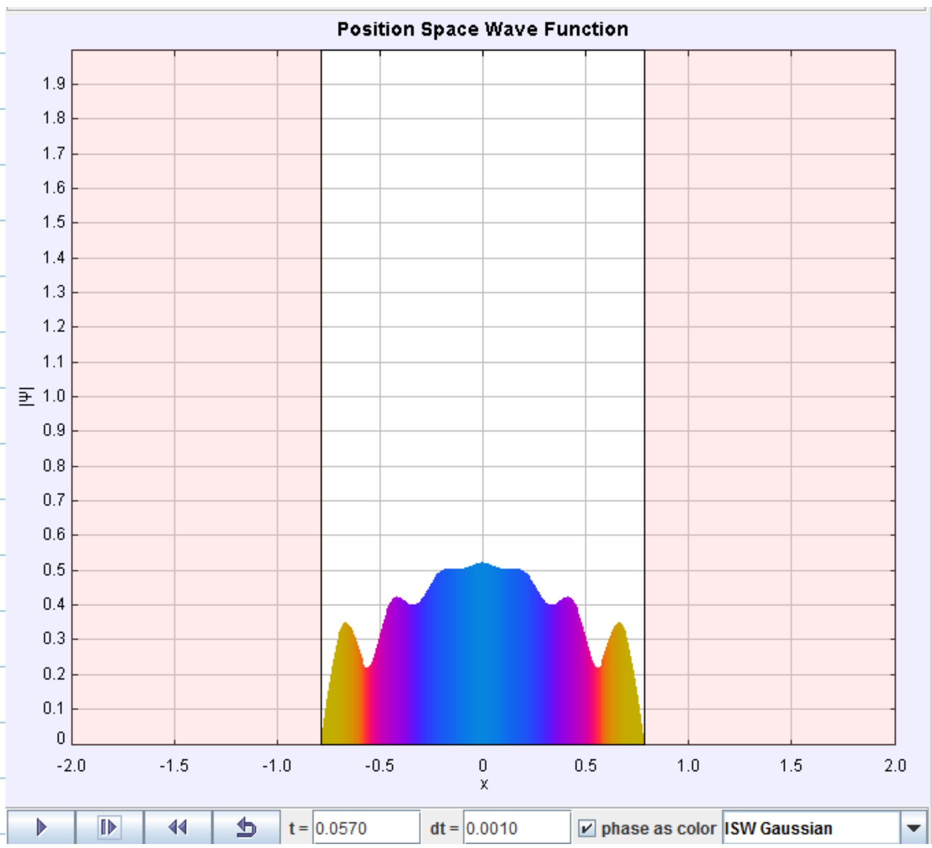
$$= \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{L}x\right)$$

7.1.5: Example of time evolution

Starting configuration

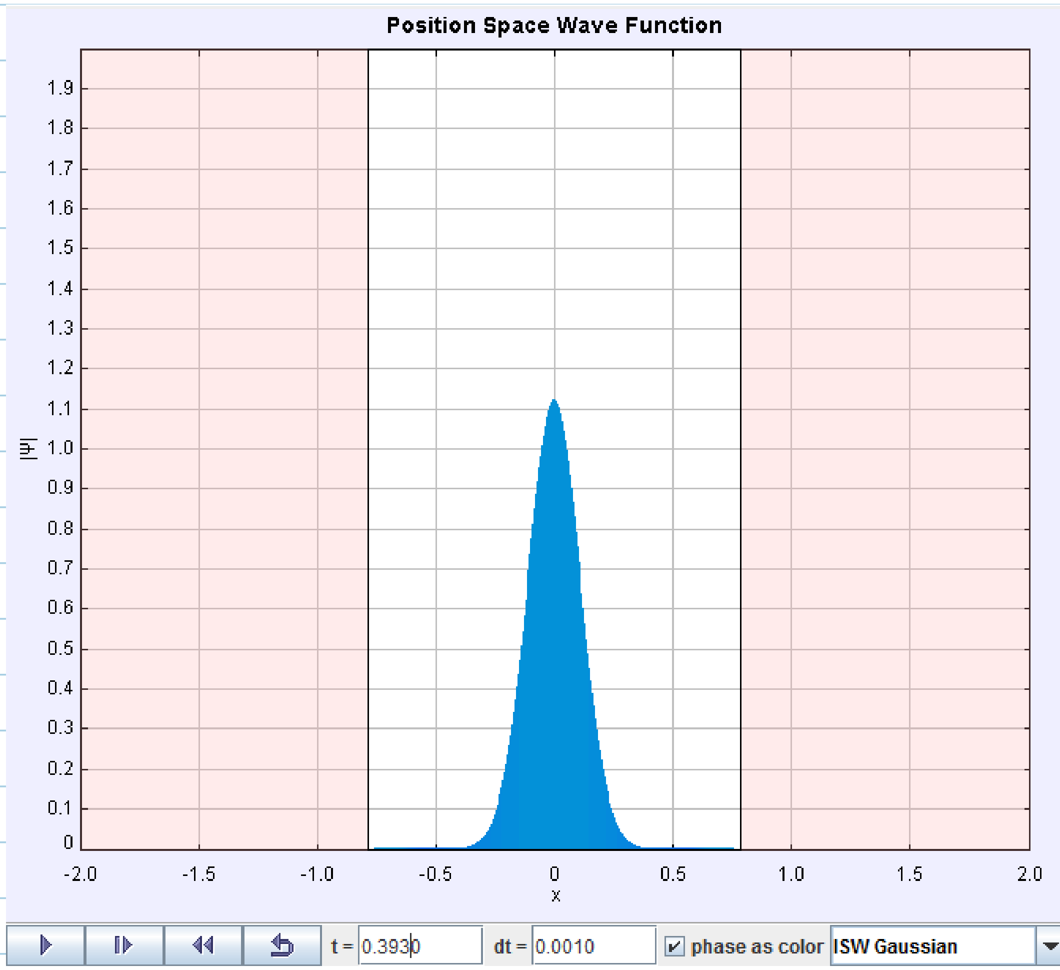


As time goes on, the wave packet first broadens, and when it flanks reach the boundary, interference effects show (wave components reflected from wall)



Note that after some time, we get the original wave packet back!

This has to do with the fact that each energy eigenstate has a phase that osciallates with some frequency, thus coming back to the orignal value. If there is only a limited number of frequencies involved, then there is some time where all of these phases of the energy eigenstates are back to the original value, thus the initial wavepacket is restored!



7.1.6 Discussion

1) Only discrete values of energy are possible for eigenstates! In general, discrete spectrum gives rise to special effects, e.g. spectroscopy of atoms

in classical mechanics: continuum of values possible

How to reconcile classical and quantum mechanics?

$$\frac{E_{n+1}-E_n}{E_n} = \frac{(n+1)^2 - n^2}{n^2} = \frac{2n+1}{n^2}$$

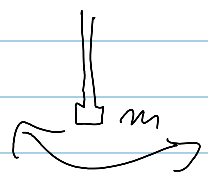
$$\lim_{n\to\infty} 1/n = 0$$

For high energies in the infinite potential well, the energy values become basically continuous.

'high energies' is defined with respect to the depth of the well ...
At room temperature, macroscopic systems are quite far from the ground state (kinetic energy related to temperature) ... Therefore quantum effects don't play a role there.

2) Quantum mechanical states that are confined energetically to some region are called **'bound states'**. These bound states always have a discrete energy spectrum!

Examples of this:
- Atomic spectrum: electron in Coulomb potential
  (Quantum Mechanics II)
- mechanical resonators



$$V(x) = \frac{1}{2} m \omega^2 x^2$$

harmonic potential (see later this lecture)

3) The ground state energy is not zero!
Ground state: state of lowest energy
==> n = 1

$$E_1 = \frac{\pi^2 \hbar^2}{2a^2 m} \quad (> 0)$$

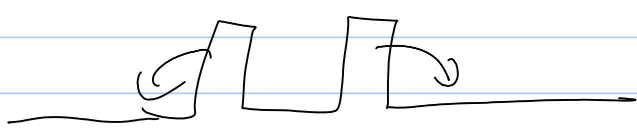
Confinement along the x-direction leads to a minimum of kinetic energy (Heisenberg Uncertainty relation) ==> therefore the term 'vacuum fluctuations"

Application: Casimir force:

- system in ground state
- force on wall?

Ground state energy would be lowered by increasing a
==> force pulls wall apart

Is that a relevant effect? Yes, in nano-mechanics
(the relevant vacuum fluctuation there are those of the electromagnetic field ...)



Structures toppled over quite often
==> explanation: electromagnetic Casimir force topples them over!