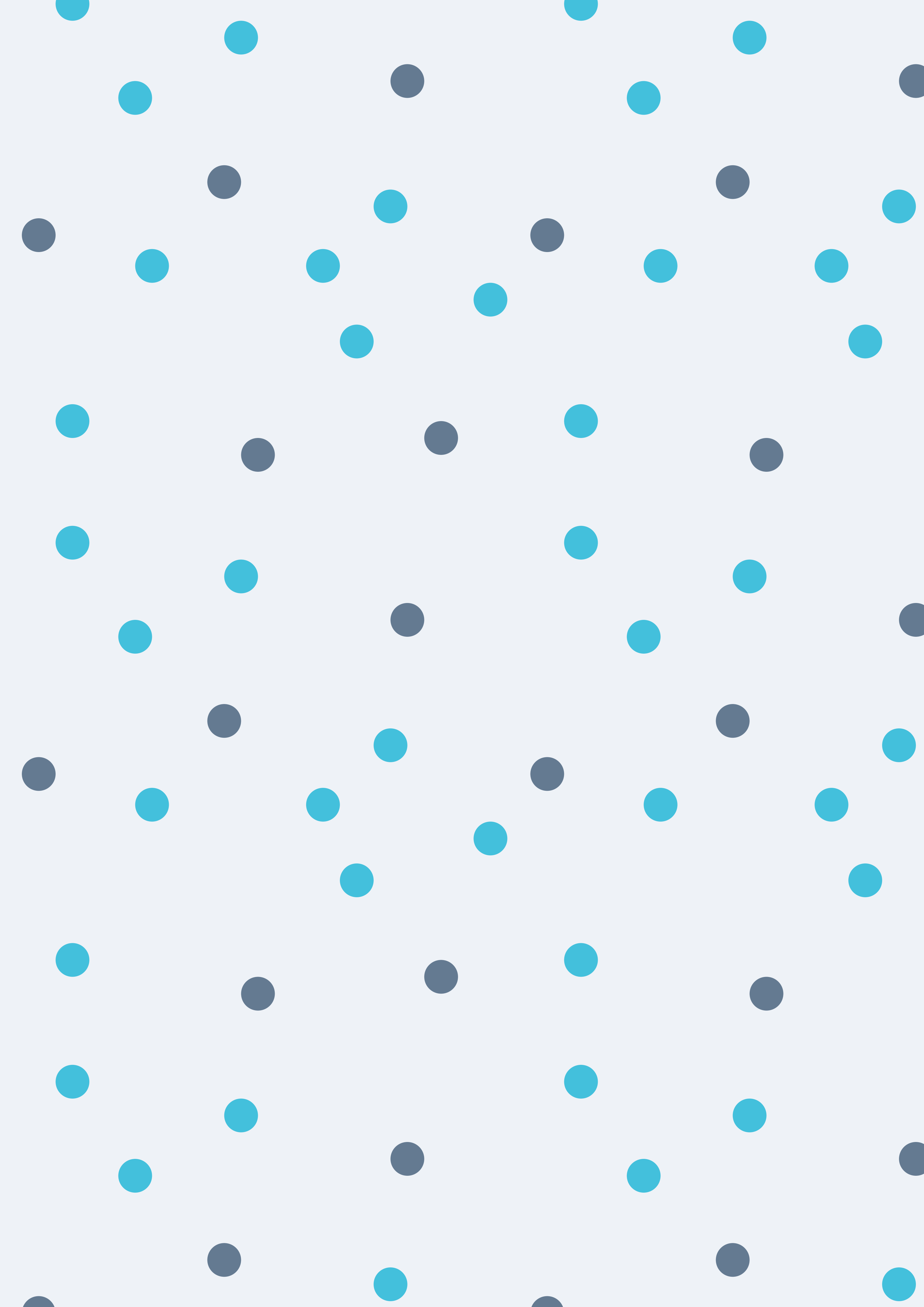


Intro to Quantum Dynamics

Trying to solve the black body problem Max Planck proposed an empirical law

Energy of light had to be quantized. This meant that light with frequency ω is emitted in packets of energy

$$E = \hbar\omega$$

▶ Planck's constant $\hbar \approx 1.05 \times 10^{-34}\ J \cdot s$

Sometimes custom to write

$$h = 2\pi\hbar$$

Louis de Broglie proposed all particles, matter and light are associated with waves, having frequency ν and wavelength λ related to energy E and momentum p of the particle through the Planck constant

$$E = h\nu \qquad p = h/\lambda$$

THE WAVEFUNCTION

Quantum mechanics tells us that light displays both wave-like and particle like properties.

Waves are different from the classical sense. They are a mathematical construct used to describe dynamics of quantum object.

Importantly the amplitude has no physical significance.

For the current description, we work in $\mathbb{R}^3$

<u>For classical</u>: state of particle at $t = t_0$ is given by position and momentum

$$\{\underbrace{\vec{x}}_{\text{position}}, \underbrace{\vec{p}}_{\text{momentum}}\}$$

and $\vec{p} = m\vec{v}$

Then $\vec{F} = m\ddot{\vec{x}}$ determines $\vec{x}$ and $\vec{v}$ for all time t

In quantum, state of particle is given by its wave function. $\psi(\vec{x},t)$

$$\boxed{\begin{aligned}\psi: \mathbb{R}^3 \times \mathbb{R} &\longrightarrow \mathbb{C} \\ (\vec{x},t) &\longmapsto \psi(\vec{x},t)\end{aligned}}$$

complex valued

The probability interpretation

Born's rule

$$P(\vec{x},t) = |\psi(x,t)|^2$$

$P(\vec{x},t)$ is the probability density

$P(\vec{x},t)$ is the probability of finding a particle at a given position

The probability of finding a particle at time t in some infitesmal volume is dV around $\vec{x}$

$$P(\vec{x},t)\,dV = |\psi(\vec{x},t)|^2$$

Therefore integrating,

$$\boxed{P_R(t) = \int_{R \subseteq \mathbb{R}^3} dV\, P(\vec{x},t) = \int_R dV\, |\psi(\vec{x},t)|^2}$$

Probability of finding a particle in a region $R \subseteq \mathbb{R}^3$

In one dimension, probability of finding a particle in an interval $[a,b]$ is

$$\boxed{P_{[a,b]} = \int_a^b dx\, P(x,t) = \int_a^b dx\, |\psi(x,t)|^2}$$

Normalisation

The particle has to be somewhere in $\mathbb{R}^3$, therefore we get normalised wave function

$$\boxed{\int_{\mathbb{R}^3} dV\, P(\vec{x},t) = \int_{\mathbb{R}^3} dV\, |\psi(x,t)|^2 dV = 1}$$

Normalised Wave function

$\psi(x,t)$

Suppose we have a non-normalised function, $\Psi(x,t)$

$$\int_{\mathbb{R}^3} dV\, |\Psi(x,t)|^2 = N < \infty$$

then we normalize it

Normalization

$$\psi(\vec{x},t) \doteq \frac{1}{\sqrt{N}}\Psi(x,t)$$

Now it is clear that a function is normalizable only if $\Psi(\vec{x},t) \longrightarrow 0$ sufficiently fast

That is if $\Psi \in L^2(\mathbb{R})$: Space of square integrable functions

Note: The phase of the wave function is totally immaterial as pertains to the probability density

$$\psi_\alpha(\vec{x},t) \doteq e^{i\alpha}\psi(\vec{x},t) \qquad \alpha \in \mathbb{R}$$

describe the same physical state. In fact $|\psi_\alpha(\vec{x},t)|^2 = |\psi(\vec{x},t)|^2 = P(\vec{x},t)$ and no other physical observable depend on α.

This is only true $\iff$ α is constant

If we multiply wave function by a spatially varying phase

$$e^{i\alpha(\vec{x})}$$

then probability density remains the same but other observables will change

Superposition

By superposition principle, if ψ_1 and ψ_2 solve the schrödinger equation then so is

$$\psi_3(\vec{x},t) = \alpha\,\psi_1(\vec{x},t) + \beta\,\psi_2(\vec{x},t) \qquad \forall\ \alpha,\beta \in \mathbb{C}$$

Additionally if $\psi_1(\underline{x},t)$ and $\psi_2(\underline{x},t)$ are possible states of a system (they are normalizable), so is $\psi_3(\vec{x},t)$.

Let

$$\int_{\mathbb{R}^3} dV\, |\psi_i(\vec{x},t)|^2 = N_i < \infty\,, \qquad i = 1,2$$

Observe

$$\begin{aligned} P_3(\underline{x},t) &= |\alpha\,\psi_1(\vec{x},t) + \beta\,\psi_2(\vec{x},t)|^2 \\ &= |\alpha|^2|\psi_1(\vec{x},t)|^2 + |\beta|^2|\psi_2(\vec{x},t)|^2 + \alpha\bar{\beta}\,\psi_1\bar{\psi}_2 + \bar{\alpha}\beta\,\bar{\psi}_1\psi_2 \qquad (A\in\mathbb{C},\ |A|^2 \doteq A\bar{A}) \\ &= |\alpha|^2 P_1 + |\beta|^2 P_2 + \alpha\bar{\beta}\,\psi_1\bar{\psi}_2 + \bar{\alpha}\beta\,\bar{\psi}_1\psi_2 \end{aligned}$$

Hence $P_3 \neq P_1 + P_2$

If ψ_1 and ψ_2 are normalizable then ψ_3 is normalizable

$$\int_{\mathbb{R}^3} |\psi_3(\vec{x},t)|^2 dV = \int_{\mathbb{R}^3} dV |\alpha\psi_1 + \beta\psi_2|^2$$

$$\leq \int_{\mathbb{R}^3} dV (|\alpha\psi_1| + |\beta\psi_2|)^2 \qquad |x+y| \leq |x| + |y|$$

$$\leq \int_{\mathbb{R}^3} dV (|\alpha\psi_1|^2 + |\beta\psi_2|^2 + 2|\alpha\psi_1||\beta\psi_1|)$$

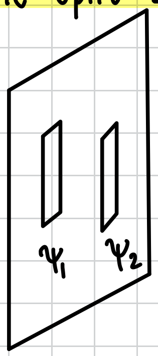
$$|x-y|^2 \geq 0 \longrightarrow |x|^2 + |y|^2 \geq 2|\alpha||y|$$

$$\leq \int_{\mathbb{R}^3} dV (2|\alpha\psi_1(\vec{x},t)|^2 + 2|\beta\psi_2(\vec{x},t)|^2)$$

$$= 2|\alpha|^2 N_1 + 2|\beta|^2 N_2 < \infty$$

showing that ψ_3 is normalizable and so represents a physical state.

Double Split Experiment



ψ_1 be the wave function of one of the slits. Similar for ψ_2.

By superposition principle,

$$\psi_3 = \psi_1 + \psi_2$$

We are adding wavefunctions - i.e. probability amplitudes, not probability densities

The probability density with both slits open is

$$|\psi_1(\vec{x},t) + \psi_2(\vec{x},t)|^2 = |\psi_1(\vec{x},t)|^2 + |\psi_2(\vec{x},t)|^2 + 2\mathrm{Re}(\overline{\psi_2(\vec{x},t)}\psi_1(\vec{x},t))$$

$$\Longrightarrow P_3(\vec{x},t) \neq P_1(\vec{x},t) + P_2(\vec{x},t)$$

In the above relation the cross term $2\mathrm{Re}(\overline{\psi_2(\vec{x},t)}\psi_1(\vec{x},t))$ is what causes the interference pattern.

SCHRÖDINGER EQUATION

Schrödinger Equation

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

- $V(\vec{x},t)$: potential energy
- plancks constant : $\hbar \approx 1.05 \times 10^{-34}$ Js

$$h = 2\pi\hbar$$

The dimensions of h is same as angular momentum $L = \vec{x} \times \vec{p}$

$$[\hbar] = [E]\cdot[T] = J\cdot s \qquad (E \equiv \text{Energy})$$

Justifying Schrödinger Equation

Assume wave function associated to a particle is a wave. In particular, a De Broglie wave.

Let ω be the frequency, wave number $\vec{k}$, E be the total energy and momentum $\vec{p}$

$$E = \hbar\omega \qquad \vec{p} = \hbar\vec{k}$$

If particle has mass m and potential $V(\vec{x},t)$

$$E = \frac{|\vec{p}|^2}{2m} + V(\vec{x},t)$$

then we get

$$\hbar\omega = \frac{\hbar^2}{2m}|\vec{k}|^2 + V \qquad (*)$$

Consider a complex harmonic wave

$$\psi_{p.w.} = Ae^{i(\vec{k}\cdot\vec{x} - \omega t)}$$

Differentiating $\psi_{p.w}$ we get

$$\omega = \frac{i}{\psi_{p.w}}\frac{\partial}{\partial t}\psi_{p.w} \qquad |\vec{k}|^2 = -\frac{1}{\psi_{p.w}}\nabla^2\psi_{p.w}$$

Substituting into $(*)$ we get

$$i\hbar\frac{\partial}{\partial t}\psi_{p.w} = -\frac{\hbar^2}{2m}\nabla^2\psi_{p.w} + V\psi_{p.w}$$

The last step is to take this expression valid for any plane waves and generalize it.

Conservation of Probability

$$\frac{\partial P(\vec{x},t)}{\partial t} = \frac{\partial}{\partial t}|\psi(\vec{x},t)|^2 = \overline{\psi(\vec{x},t)}\frac{\partial}{\partial t}\psi(\vec{x},t) + \psi(\vec{x},t)\frac{\partial}{\partial t}\overline{\psi(\vec{x},t)}$$

From Schrödinger equation we find (taking complex conjugate)

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

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

Remark: Potential $V(\vec{x},t)$ always assumed to be real.

Substituting,

$$\frac{\partial P(\vec{x},t)}{\partial t} = \left[\overline{\psi}\frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\underline{\nabla}^2\psi + V\psi\right) - \psi\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\underline{\nabla}^2\overline{\psi} + V\overline{\psi}\right)\right]$$

$$= \left[\cancel{\frac{1}{i\hbar}V|\psi|^2} - \cancel{\frac{1}{i\hbar}V|\psi|^2} - \frac{1}{i\hbar}\frac{\hbar^2}{2m}\overline{\psi}\underline{\nabla}^2\psi + \frac{1}{i\hbar}\frac{\hbar^2}{2m}\psi\underline{\nabla}^2\overline{\psi}\right]$$

$$= \frac{\hbar}{2im}\left(\psi\underline{\nabla}^2\overline{\psi} - \overline{\psi}\underline{\nabla}^2\psi\right)$$

Define

$$\boxed{\vec{J}(\vec{x},t) = -\frac{i\hbar}{2m}\left(\overline{\psi(\vec{x},t)}\,\underline{\nabla}\,\psi(\vec{x},t) - \psi(\vec{x},t)\,\underline{\nabla}\,\overline{\psi(\vec{x},t)}\right)}$$

Probability current

Note: The divergence of $\vec{J}$ is

$$\underline{\nabla}\cdot\underline{J} = \underline{\nabla}\cdot\left[-\frac{i\hbar}{2m}\left(\overline{\psi(\vec{x},t)}\,\underline{\nabla}\,\psi(\vec{x},t) - \psi(\vec{x},t)\,\underline{\nabla}\,\overline{\psi(\vec{x},t)}\right)\right]$$

$$= \frac{-i\hbar}{2m}\left(\overline{\psi}\underline{\nabla}^2\psi - \psi^2\underline{\nabla}^2\overline{\psi} + \cancel{\underline{\nabla}\overline{\psi}\cdot\underline{\nabla}\psi} - \cancel{\underline{\nabla}\psi\cdot\underline{\nabla}\overline{\psi}}\right)$$

$(\nabla^2 f = \underline{\nabla}\cdot\underline{\nabla}(f))$

Therefore we get

$$\boxed{\frac{\partial}{\partial t}P(\vec{x},t) + \underline{\nabla}\cdot\vec{J}(\vec{x},t) = 0}$$

Flux of Probability

Computing probability in a region $R \subset \mathbb{R}^3$; $P_R(t)$

$$P_R(t) = \int_R dV\, P(\vec{x},t)$$

By the above, we get

$$\frac{d}{dt} P_R(t) = \int_R dV\, \partial_t P(\vec{x},t) = -\int_R dV\, \underline{\nabla} \cdot \vec{J}(\vec{x},t)$$

$$= -\int_{\partial R} d\underline{S} \cdot \vec{J}(\vec{x},t) \qquad \text{Gauss' Divergence theorem}$$

We see that the probability that particle lies in R can change only if there is a flow of probability through the surface ∂R that bounds R

If $\vec{J}=0$ on ∂R or R has no bounds, then probability that particle is in region R is time independent.

If we consider $R=\mathbb{R}^3 \Longrightarrow \partial R = S^2_\infty$. We should have

$$\int_{\mathbb{R}^3} dV |\psi(\vec{x},t)|^2 < \infty \iff \psi(\vec{x},t) \longrightarrow 0 \text{ as } |\vec{x}| \to \infty$$

$$\iff \psi \in L^2(\mathbb{R}^3)$$

We need

$$\int_{S^2_\infty} dS \cdot \vec{J}(\vec{x},t) = 0 \Longrightarrow \frac{\partial}{\partial t} P_{\mathbb{R}^3} = 0$$

Remarks:

1) The operator $\hat{H}$ is Hamiltonian operator defined as

$$\boxed{\hat{H}(\vec{x},t) \doteq -\frac{\hbar^2 \nabla^2}{2m} + V(\vec{x},t)} \qquad \text{Hamiltonian Operator}$$

Different choices of Hamiltonian describes different laws of physics

In particular, the Schrödinger equation is only valid for non-relativistic particles, i.e. when velocity of particles much less than speed of light.

2) General Schrödinger Equation

$$\boxed{i\hbar \frac{\partial}{\partial t} \psi(\vec{x},t) = \hat{H}(\vec{x},t)\,\psi(\vec{x},t)}$$

3) Energy in classical is

$$E_{cl} = \frac{|\vec{p}|^2}{2m} + V(\vec{x})$$

To get energy in quantum, do quantization. Take maps

$$\boxed{\begin{aligned} \vec{p} &\longrightarrow i\hbar \underline{\nabla} \\ E_{cl} &\longrightarrow \hat{H} \end{aligned}}$$

Quantization and Observables

In classical, state of a particle is described by position $\vec{x}$ and momentum $\vec{p}$

$\{\vec{x}, \vec{p}\}$: observables

$F(\vec{x},\vec{p})$ is a classic observable

In quantum, state of particle is encoded by it's wave function which gives a probability density

$$P(\vec{x},t) = |\psi(\vec{x},t)|^2$$

Since we do not have certainty, we cannot really speak of a value of the position. In the probability setting, we use the mean value

$$\boxed{\langle \vec{x} \rangle \doteq \int_{\mathbb{R}^3} dV\, \vec{x}\, |\psi(\vec{x},t)|^2 = \int_{\mathbb{R}^3} dV\, \overline{\psi}(\vec{x},t)\, \vec{x}\, \psi(\vec{x},t)}$$ Mean Value of position

Remark: This is basically the formula for expectation value

Looking at momentum;

$$\langle \vec{p} \rangle = \int_{\mathbb{R}^3} dV\, \vec{p}\, |\psi(\vec{x},t)|^2$$

We must determine the $\vec{x}$ dependence in order to perform the integral.

Remember the trick used to justify Schrödinger Equation

$$\psi_{p.w}(\vec{x},t) = Ae^{i(1/\hbar\, p\cdot\vec{x} - \omega t)} \implies \vec{p}\,\psi_{p.w}(\vec{x},t) = i\hbar \underline{\nabla} \psi_{p.w}(\vec{x},t)$$

and suppose this holds for any generic wave function

$$\boxed{\hat{\vec{p}}\,\psi(\vec{x},t) \doteq -i\hbar\,\underline{\nabla}\,\psi(\vec{x},t)}$$

where $\hat{\vec{p}}$ is the momentum operator. Now

$$\boxed{\langle\hat{\vec{p}}\rangle \doteq \int_{\mathbb{R}^3} dV\,\overline{\psi}(x,t)\,\hat{p}\,\psi(x,t) \equiv -i\hbar\int_{\mathbb{R}^3} dV\,\overline{\psi}(\vec{x},t)\,\underline{\nabla}\,\psi(\vec{x},t)}$$

Therefore in quantum, momentum is not a vector but an operator

We cannot think of momentum $\vec{p}$ as an observable in the classical sense.

> In quantum mechanics, observables are operators acting on wavefunctions

In general

$$\boxed{\begin{gathered} O_{cl}(\vec{x},\vec{p}) \longrightarrow \hat{O} \doteq O_{cl}(\hat{x},\hat{p}) \\ \langle\hat{O}\rangle = \int_{\mathbb{R}^3} dV\,\overline{\psi}(\vec{x},t)\,\hat{O}\cdot\psi(x,t) \end{gathered}}$$

This procedure is called quantization

As we saw above, operators for momentum and position are

$$\boxed{\hat{\vec{x}}\cdot\psi(\vec{x},t) = \vec{x}\,\psi(\vec{x},t) \qquad \hat{\vec{p}}\cdot\psi(\vec{x},t) = -i\hbar\,\underline{\nabla}\,\psi(\vec{x},t)}$$

Examples:

1) $E(\vec{x},\vec{p}) \xrightarrow[\text{quant.}]{} \hat{H} = \dfrac{|\hat{\vec{p}}|^2}{2m} + V(\hat{x},t)$

$$\hat{H}\,\psi(\vec{x},t) = \left[-\frac{\hbar}{2m}\underline{\nabla}^2 + V(\vec{x},t)\right]\psi(\vec{x},t)$$

2) In classical, angular momentum is

$$L_{cl} = \vec{x}\times\vec{p}$$

By quantization,

$$L_{cl} = \vec{x}\times\vec{p} \xrightarrow[\text{quant.}]{} \hat{\underline{L}} = \hat{\vec{x}}\times\hat{\vec{p}}$$

$$\hat{\underline{L}}\cdot\psi(\vec{x},t) = \hat{\vec{x}}\times\left(-i\hbar\,\underline{\nabla}\,\psi(\vec{x},t)\right)$$

To see this, consider first component of angular momentum L_1. By defn of cross product

$$L_1 = x_2 p_3 - x_3 p_2 \longrightarrow \hat{L}_1 = \hat{x}_2 \hat{p}_3 - \hat{x}_3 \hat{p}_2$$

$$\begin{aligned}
\hat{L}_1 \psi(\vec{x},t) &= (\hat{x}_2 \hat{p}_3 - \hat{x}_3 \hat{p}_2) \psi(\vec{x},t) \\
&= \hat{x}_2 \hat{p}_3 \psi(\vec{x},t) + \hat{x}_3 \hat{p}_2 \psi(\vec{x},t) \\
&= \hat{x}_2 \left(-i\hbar \frac{\partial}{\partial x_3} \psi \right) + \hat{x}_3 \left(-i\hbar \frac{\partial}{\partial x_2} \psi(x,t) \right) \\
&= \hat{x}_2 \phi(\vec{x},t) + \hat{x}_3 \eta(\vec{x},t) \\
&= x_2 \phi(\vec{x},t) + x_3 \eta(\vec{x},t) \\
&= x_2 \left(-i\hbar \frac{\partial}{\partial x_3} \psi \right) + x_3 \left(-i\hbar \frac{\partial}{\partial x_2} \psi \right)
\end{aligned}$$

where we defined

$$\phi(\vec{x},t) = -i\hbar \frac{\partial}{\partial x_3} \psi \qquad \eta(\vec{x},t) = -i\hbar \frac{\partial}{\partial x_2} \psi(x,t)$$

Note: In general operators do NOT commute

In 1D: Wavefunction $\psi(x,t)$

$$\hat{p} \cdot \psi(x,t) = i\hbar \frac{\partial}{\partial x} \psi(x,t)$$

$$\hat{x} \cdot \psi(\vec{x},t) = x \psi(x,t)$$

$$\begin{aligned}
(\hat{p} \cdot \hat{x} - \hat{x} \cdot \hat{p}) \psi(\vec{x},t) &= \hat{p} \cdot (x\psi) + i\hbar \hat{x} \cdot \left(\frac{\partial}{\partial x} \psi \right) \\
&= -i\hbar \frac{\partial}{\partial x} (x \psi(x,t)) + i\hbar x \frac{\partial}{\partial x} \psi(x,t) \\
&= -i\hbar \left(x \frac{\partial}{\partial x} \psi + \psi \right) + i\hbar x \frac{\partial}{\partial x} \psi(x,t) \\
&= -i\hbar \psi(\hat{x},t)
\end{aligned}$$

Commutator: $[A,B] = \hat{A}\hat{B} - \hat{B}\hat{A}$

$$[\hat{x}, \hat{p}] = -i\hbar$$

True when acting on functions of x

Poisson brackets $\{x,p\}_{P.B} = 1$

Heisenberg Uncertainty Principle

Variance

Basically tells us how much the probability distribution of the observable $\mathcal{O}$ is spread around its mean value.

$$\text{Variance}: (\Delta O)^2 = \langle(\hat{O} - \langle\hat{O}\rangle)^2\rangle$$
$$= \langle\hat{O}^2 - 2\hat{O}\langle\hat{O}\rangle + \langle\hat{O}\rangle^2\rangle$$
$$= \langle\hat{O}^2\rangle - 2\langle\hat{O}\langle\hat{O}\rangle\rangle + \langle\langle\hat{O}\rangle^2\rangle \qquad \text{Linearity of Expectation}$$
$$= \langle\hat{O}^2\rangle - 2\langle\hat{O}\rangle^2 + \langle\hat{O}\rangle^2 \qquad \langle\hat{O}\rangle \text{ is just a number}$$

$\Rightarrow$ **Variance** $\boxed{(\Delta O)^2 = \langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2}$

Heisenberg Uncertainty Principle

There is a limit to the precision with which pairs of physical properties e.g position and momentum can be simultaneously known.

In other words, the more accurately one is measured, the less accurately the other can be known.

For position and momentum, this is expressed by

$$\boxed{\Delta x \, \Delta p \geq \frac{\hbar}{2}}$$

Proof: Dropping the explicit dependence on t.

Consider the 1D family of wave functions

$$\Psi_s(x) = (\hat{p} - is\hat{x})\,\psi(x) \qquad s \in \mathbb{R}$$

for some reference wavefunction $\psi(x)$.

$\Psi_s(x)$ are bonafide states $\Longrightarrow$ they are positive definite

$$\int_{\mathbb{R}} dx\, |\Psi_s(x)|^2 \geq 0$$

Therefore we get

$$0 \leq \int_{\mathbb{R}} dx\, (\hat{p}-is\hat{x})\cdot \overline{\psi}(x)(\hat{p}-is\hat{x})\,\psi(x)$$

$$= \int_{\mathbb{R}} dx \overline{\left(-i\hbar\partial_x\psi(x) - isx\,\psi(x)\right)}\left(-i\hbar\partial_x\psi(x) - isx\,\psi(x)\right)$$

$$= \int_{\mathbb{R}} dx \left[\hbar^2 (\overline{\partial_x\psi})(\partial_x\psi) + \hbar s x \overline{\partial_x\psi}\,\psi + \hbar s \partial_x\psi\,\overline{\psi} + s^2 x^2 \overline{\psi}\psi\right]$$

integration by parts

$$= \int_{\mathbb{R}} dx \left[\underbrace{-\hbar\overline{\psi}(x)\psi''(x)}_{\overline{\psi}(-i\hbar)^2\partial_x^2\psi} - \hbar s \overline{\psi}\underbrace{\partial_x(x\psi)}_{|\psi|^2 + x\overline{\psi}\partial_x\psi} + \hbar s x(\partial_x\psi)\overline{\psi} + s^2x^2|\psi|^2\right]$$

$$\overline{\psi}\,\hat{p}^2\,\overline{\psi} \qquad -i\hbar\partial_x\psi = \hat{p}\psi \implies \partial_x\psi = \frac{i}{\hbar}\hat{p}\psi$$

$$= \int_{\mathbb{R}} dx \left[\overline{\psi}\hat{p}^2\psi - \hbar s|\psi|^2 \cancel{- isx\overline{\psi}\hat{p}\psi + isx\overline{\psi}\hat{p}\psi} + s^2x^2|\psi|^2\right]$$

$$= \int_{\mathbb{R}} dx \left[\overline{\psi}\hat{p}^2\psi - \hbar s|\psi|^2 + s^2x^2|\psi|^2\right]$$

$$= \langle \hat{p}^2\rangle - \hbar s + s^2\langle\hat{x}^2\rangle \qquad \int_{\mathbb{R}} |\psi|^2 = \langle 1\rangle \equiv 1$$

Make the following assumptions

$\langle\hat{x}\rangle = 0$

$\langle\hat{p}\rangle = 0$

if not, redefine

$\hat{x} \longrightarrow \hat{x} - \langle\hat{x}\rangle$

$\hat{p} \longrightarrow \hat{p} - \langle\hat{p}\rangle$

We then get $\quad (\Delta x)^2 = \langle\hat{x}^2\rangle \qquad (\Delta p)^2 = \langle\hat{p}^2\rangle$

Hence

$$0 \leq \langle\hat{p}^2\rangle - \hbar s + s^2\langle\hat{x}^2\rangle$$
$$= (\Delta p)^2 + s^2(\Delta x)^2 - s\hbar \qquad \forall s\in\mathbb{R}$$

This is only true if right-hand side has one or zero roots $\implies$ discriminant non-positive

$$\hbar^2 - 4(\Delta x)^2(\Delta y)^2 \leq 0 \implies \Delta x\Delta p \geq \frac{\hbar}{2}$$

■

Example : Gaussian Wave Packet

Consider the following normalised guassian state

$$\psi(x) = \left(\frac{a}{\pi}\right)^{\frac{1}{4}} e^{-\frac{ax^2}{2}}$$

Aside:

$$I = \int_{-\infty}^{\infty} dx\, e^{-ax^2} \implies I^2 = \left(\int_{-\infty}^{\infty} dx\, e^{-ax^2}\right)^2 = \int_{-\infty}^{\infty} dx\, e^{-ax^2} \int_{-\infty}^{\infty} dy\, e^{-ay^2}$$

$$= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\, e^{-a(x^2+y^2)}$$

using polar substitution

$$x = r\cos\theta \quad y = r\sin\theta$$

New bounds of integration:

$$0 \leq r \leq \infty$$

$$0 \leq \theta \leq 2\pi$$

$$I^2 = \int_0^{2\pi} d\theta \int_0^{\infty} dr\, \underset{\text{Jacobian}}{r}\, e^{-ar^2} = \frac{\pi}{a} \implies I = \left(\frac{\pi}{a}\right)^{1/2}$$

Hence

$$\int_{\mathbb{R}} dx\, |\psi(x)|^2 = 1$$

Important !

$$I_m(a) = \int_{-\infty}^{\infty} dx\, x^{2m} e^{-ax^2} = \int_{-\infty}^{\infty} dx \left(-\frac{d}{da}\right)^m e^{-ax^2}$$

$$= \left(-\frac{d}{da}\right)^m \sqrt{\frac{\pi}{a}}$$

Computing mean values

1) $\langle \hat{x} \rangle = \int_{\mathbb{R}} dx\, \overline{\psi}(x)\, \hat{x}\, \psi(x) = \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, x e^{-ax^2} = 0$

2) $\langle \hat{p} \rangle = \int_{\mathbb{R}} dx\, \overline{\psi}\, \hat{p}\, \psi(x) = -i\hbar \sqrt{\frac{a}{\pi}} \int_{\mathbb{R}} dx \left(-\frac{a}{2}\right) 2x e^{-ax^2} = 0$

Computing uncertainties

1) $\langle \hat{x}^2 \rangle = \sqrt{\frac{a}{\pi}} \int_{\mathbb{R}} dx\, x^2 e^{-ax^2} = -\sqrt{\frac{a}{\pi}} \frac{d}{da} \int_{\mathbb{R}} dx\, e^{-ax^2} = -\sqrt{\frac{a}{\pi}} \frac{d}{da} \sqrt{\frac{a}{\pi}} = \frac{1}{2a}$

2) $\langle \hat{p}^2 \rangle = (i\hbar)^2 \sqrt{\frac{a}{\pi}} \int_{\mathbb{R}} dx\, a^{-\frac{ax^2}{2}} \frac{\partial^2}{\partial x^2} e^{-ax^2/2}$

$= -\hbar^2 \sqrt{\frac{a}{\pi}} \left[-\int_{\mathbb{R}} dx\, a e^{-ax^2} + \int_{\mathbb{R}} dx\, a^2 x^2 e^{-ax^2} \right]$

$= -\hbar^2 \sqrt{\frac{a}{\pi}}\, a(-\hbar^2) \sqrt{\frac{a}{\pi}} = \frac{\hbar a}{2}$

$\frac{\partial}{\partial x} e^{-\frac{ax^2}{2}} = -\frac{a}{2} 2x e^{-ax^2/2}$

$\frac{\partial^2}{\partial x^2} e^{-\frac{ax^2}{2}} = -a e^{-\frac{ax^2}{2}} + a^2 x^2 e^{-\frac{ax^2}{2}}$

We see that

$\Delta x \Delta p = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} = \frac{\hbar}{2}$

SOLVING SCHRÖDINGER EQUATION

Focusing on 1D

Time independent Schrödinger Equation

Assume $V(x)$ to be static, i.e. time independent

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

1D Schrödinger Equation

time independent potential

Seperation of Variables

$$\psi(x,t) = u(x)T(t)$$

Plugging ansatz in Schrödinger Equation and dividing both sides by

$$i\hbar \frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m}\frac{u''(x)}{u(x)} + V(x) \equiv E$$ energy constant

$$\Longrightarrow T'(t) = \frac{-i}{\hbar}E(t)\,T(t) \Longrightarrow \boxed{T(t) = Ce^{-i\frac{E}{\hbar}t}}$$ where $C = T(0)$

Set $C=1$, we get

$$\boxed{\psi(x,t) = e^{-i\frac{E}{\hbar}t}u(x)}$$

Here $u(x)$ is the solution to the time-independent Schrödinger Equation

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

stationary states have definite energy E

$$\Delta E = 0 \quad \begin{cases} \psi(x,t) = u(x)e^{-\frac{iE}{\hbar}t} \\ \hat{H}\psi(x,t) = E\psi(x,t) \end{cases}$$ *

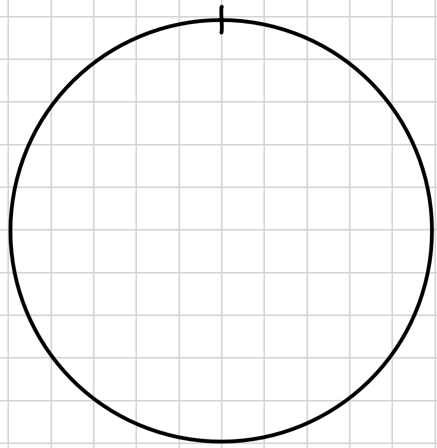
We can rewrite above as using Hamiltonian operator

$$\boxed{\hat{H}(x)u(x) = Eu(x)} \qquad \hat{H}(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Resembles eigenvalue problem $\Longrightarrow$ admits solutions for specific values of E

$\Longrightarrow$ energy quantized and solutions called stationary states

Particle on a circle



Focus particle on a compact space: S^1

$$S^1 \qquad x \sim x + 2\pi R$$

There is no potential $\Longrightarrow$ $V(x) = 0$

Therefore the time independent equation becomes

$$-\frac{\hbar^2}{2m} u''(x) = E u(x)$$

$$\Rightarrow \quad u''(x) = -\frac{2mE}{\hbar^2} u(x) \longrightarrow \boxed{u(x) = Ae^{ikx}} \quad A \in \mathbb{C} \qquad k^2 = \frac{2mE}{\hbar^2}$$

Particle lives on a circle, so imposing periodicity condition (boundary condition)

$$u(x + 2\pi R) = u(x) \Longrightarrow \boxed{k = \frac{n}{R}}, \; n \in \mathbb{Z} \qquad \text{quantization condition}$$

Therefore both momentum and Energy can only take discrete forms

$$\boxed{p_n = \frac{\hbar}{R} n \qquad E_n = \frac{\hbar^2}{2mR^2} n^2 \qquad n \in \mathbb{Z}}$$

The collection of energies is called a spectrum of the Hamiltonian

For $n=0$, $u_0(x)$ is called the ground state

$n \neq 0$: excited states

Classical limit

Quantum theory contains classical, so we need a way of recovering classical mechanics.

We need to be able to recover classical expressions and expectations from quantum formulae. We achieve this by the limit

$$\hbar \longrightarrow 0 \qquad \text{classical limit}$$

$\hbar$ is a universal constant. So $\hbar \to 0$ does not make sense. Practically this means when taking the classical limit, we assume $\hbar$ is very small compared to the system scale.

In the circle example, these are radius R and mass m and we say

$$mR^2 \gg \hbar^2$$

The relative energy levels become

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

become very small and energy become small.

Also true if n becomes large.

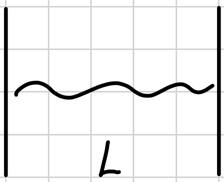
Continuing analysis of particle in a circle, we need to ensure wave function is correctly normalized.

$$\int_0^{2\pi R} dx\,|u(x)|^2 = 2\pi R|A|^2 = 1 \qquad \text{(when } n=0\text{)}$$

fix $A = \frac{1}{2\pi R}$. Then

$$u_n(x) = \frac{e^{ikx}}{\sqrt{2\pi R}} \qquad n \in \mathbb{Z}$$

Particle in a box



Consider particle confined in interval $x \in (0, L)$

Achieve this with infinite potential well

$$V(x) = \begin{cases} 0 & 0<x<L \\ \infty & \text{otherwise} \end{cases} \implies u=0$$

We are dealing with a free particle, even though we introduced a potential.

Schrödinger equation splits into two

$$u(x)V(x) = \begin{cases} -\frac{\hbar^2}{2m}u''(x) = E\,u(x) & 0<x<L \\ \lim_{V\to\infty}\left[-\frac{\hbar}{2m}u''(x) + (V-E)u(x)\right] = 0 & \text{otherwise} \end{cases}$$

imposing boundary condition

$$\lim_{x\searrow 0} u(x) = \lim_{x\nearrow 0} u(x) = 0, \qquad u(0)=0, \quad u(L)=0$$

we need wavefunction to vanish identically at infinite potentials

$$u(x) = \begin{cases} u(x) & 0<x<L \\ 0 & \text{otherwise} \end{cases}$$

The general solution is

$$u_k(x) = Ae^{ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar} > 0 \qquad x \in (0, L)$$

By superposition principle (to satisfy boundary condition $u(0) = 0$)

$$u(x) = u_k(x) + u_{-k}(x) \implies u(x) = A e^{ikx} + Be^{-ikx}$$

Applying boundary condition,

1) $u(0) = 0 \implies A + B = 0 \implies B = -A$

2) $u(L) = 0 \implies A(e^{ikL} - e^{-ikL}) = 2i A\sin(kL) = 0$

$$\implies kL = n\pi$$

$$\implies k = \frac{n\pi}{L} \qquad n \in \mathbb{N}$$

$$\boxed{u_n(x) = A\sin\left(\frac{\pi}{L} n x\right)}$$

Normalization: We require

$$\int_0^L |u_n(x)|^2 = 1 \implies A^2 \int_0^L \sin^2\left(\frac{\pi}{L} n x\right) dx = 1$$

$$\implies A^2 \frac{L}{2} = 1$$

$$\implies A = \sqrt{\frac{2}{L}}$$

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

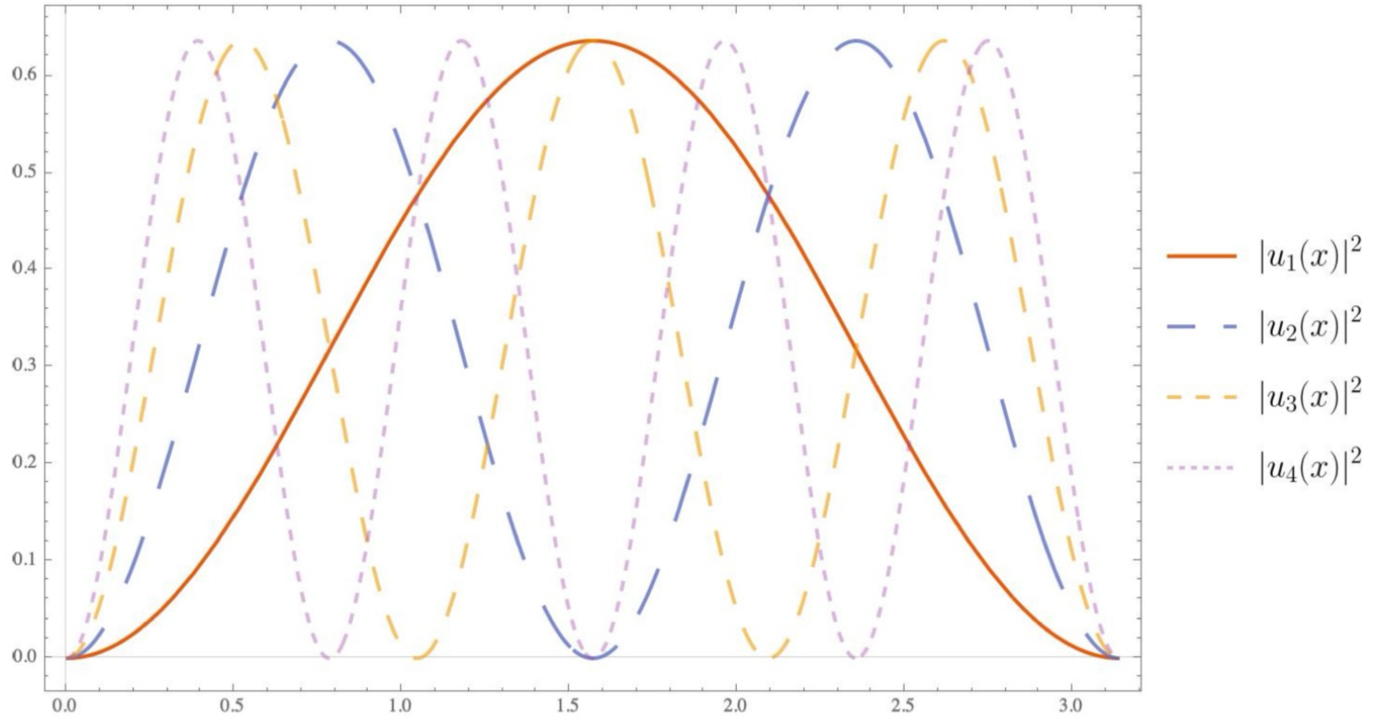
Expression for energy is

$$\boxed{E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2 \qquad n \in \mathbb{N}}$$

The probability densities of the stationary states are

$$|u_n(x)|^2 = \frac{2}{L}\left[\sin\left(\frac{\pi}{L} n x\right)\right]^2, \qquad n \in \mathbb{N}$$

below, we plot graphs



Probability densities for a particle in a box of length $L = \pi$.

As n increases, energy increases the particle is more and more likely to be found at n seperate points where $|u_n(x)|^2$ exhibits maxima.

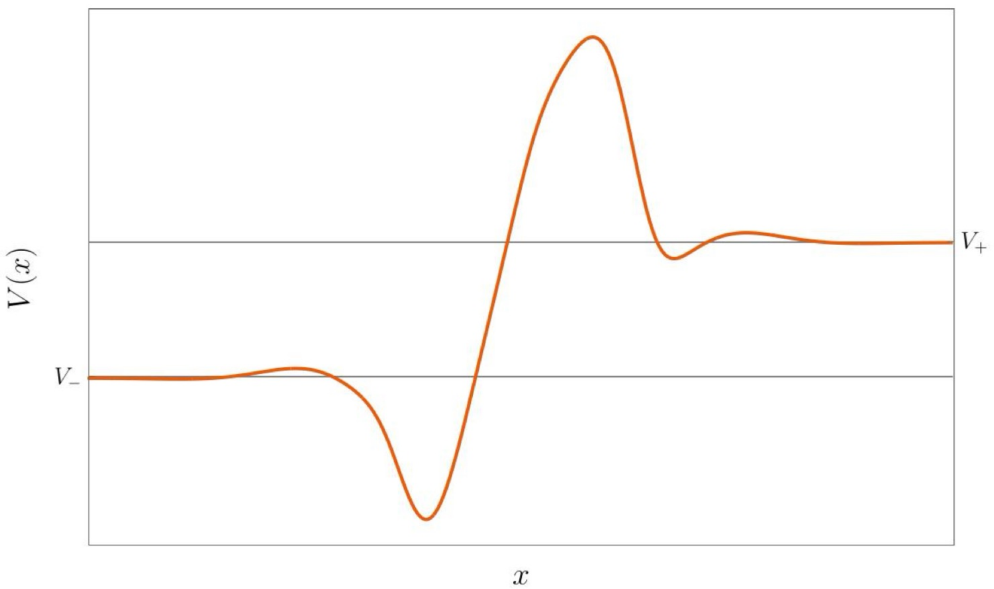
Classical limit is achieved when $m/\hbar^2$ is very large.

BOUNDED AND BOUNCED PARTICLES

Studying potentials that asymptote to a constant value.

$$\lim_{x \to \pm\infty} V(x) = V_{\pm} < \infty$$

The following is an example function



Our potential needs to decay sufficiently fast.

When x is large, $x \to \pm\infty$

$$-\frac{\hbar^2}{2m} u''(x) \approx (E - V_\pm) u(x) \quad , \quad x \longrightarrow \pm\infty$$

Particle approximately free at large distances. There are 2 qualitatively different solutions:

1) $E - V_\pm > 0$: Scattering states

In this case, wave functions are characterized by $k_\pm \in \mathbb{R}$ and behave asymptotically as complex exponentials

$$\boxed{u(x) \underset{x\to\pm\infty}{\sim} a e^{ik_\pm x} \qquad E - V_\pm = \frac{\hbar^2}{2m} k_\pm^2} \qquad x \to \pm\infty$$

2) $E - V_\pm < 0$: Bound State

In this case, wave functions are characterized by $\eta_\pm \in \mathbb{R}$ and take asymptotically form of real exponentials

$$\boxed{u(x) \underset{x\to\pm\infty}{\sim} A e^{\eta_\pm x} + B e^{-\eta_\pm x} \qquad E - V_\pm = -\frac{\hbar^2}{2m} \eta_\pm^2} \qquad x \to \pm\infty$$

Note: Neither

$$\psi_{s.c}(x, k) = a e^{ikx} \quad \text{and} \quad \psi_{b.s} = A e^{\eta x} + B e^{-\eta x}$$

are wave functions, they are both non-normalizable

Bound State

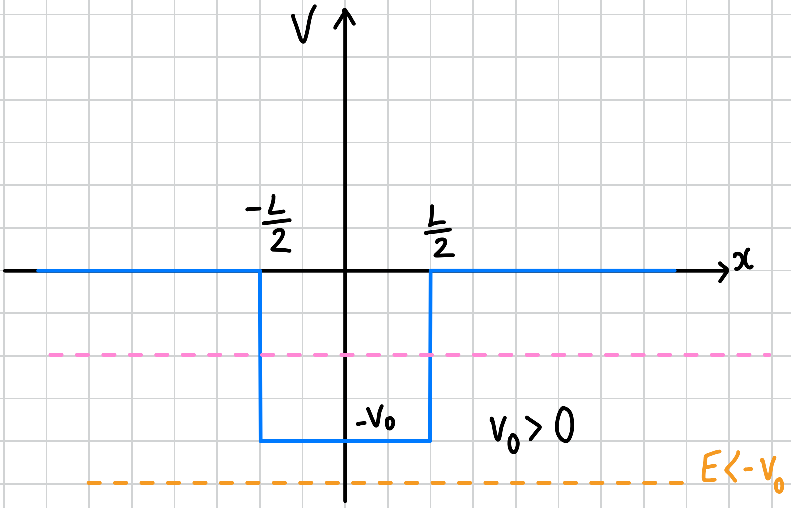
To solve the issue of non-normalization, we solve this by requiring that the full solution to the Schrödinger equation be

$$\boxed{u(x) \approx \begin{cases} B e^{-|\eta_+| x} & x \longrightarrow +\infty \\ A e^{|\eta_-| x} & x \to -\infty \end{cases}} \qquad \text{Bound States}$$

For scattering states we need to be more careful.

Potential Well: Finite Well

Consider a finite and symmetric well



$$V(x) = \begin{cases} -V_0 & -\frac{L}{2} < x < \frac{L}{2} \\ 0 & \text{otherwise} \end{cases}$$

The Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} u''(x) = \begin{cases} (E + V_0)u(x) & -\frac{L}{2} < x < \frac{L}{2} \\ E u(x) & \text{otherwise} \end{cases}$$

Clearly $u''(x)$ is discontinuous. We want $u(x)$ to be continuous

Integrating around interval $(-L/2 - \varepsilon, L/2 + \varepsilon)$

$$\frac{-\hbar^2}{2m} \int_{-\frac{L}{2}-\varepsilon}^{\frac{L}{2}+\varepsilon} dx\, u''(x) = \int_{-L/2-\varepsilon}^{L/2+\varepsilon} dx (E - V(x)) u(x)$$

In the limit $\varepsilon \to 0$ LHS becomes $-\hbar^2/2m\, u(-L/2)$ and RHS is finite since it the integral of a piecewise constant.

$$\implies u(x) \in C^1$$

$\implies$ continuously once differentiable

We want bound state solutions, when: $E < V_\pm = 0$

Note: NO non-zero solutions for $E < -V_0$ as wave function vanishes identically

Here $u(x) = ae^{\eta x} + be^{-\eta x}$ inside and outside the well where

$$\left. \begin{array}{l} u \underset{x\to\infty}{\sim} 0 \\ u \underset{x\to-\infty}{\sim} 0 \end{array} \right\} \implies u(x) = 0$$

and $u(x) = ae^{\eta x} + be^{-\eta x}$ is not normalizable.

Hence solution inside well is a sum of complex exponentials

Observation: V is symmetric hence

$V(-x) = V(x) \implies$ if $u(x)$ is a solution with energy E, then $u(-x)$ is also a solution with energy E.

Assume no two distinct state possess the same energy

Assuming for each energy E, $\exists$ 1 single state, we get

$$\left.\begin{aligned} u(x) &= \alpha u(-x) \\ u(x) &= \alpha u(-x) = \alpha^2 u(-(-x)) \equiv \alpha^2 u(x) \end{aligned}\right\} \Longrightarrow \alpha = \pm 1$$

Therefore we have 2 classes of solutions

1) even: $u(x) = u(-x)$
2) odd: $u(x) = -u(-x)$

Even Case

Outside well

- $x > \frac{L}{2}$: $u(x) = Ae^{-\eta x}$ $\quad \eta^2 = -\frac{2mE}{\hbar^2}$
- $x < -\frac{L}{2}$ $\quad u(x) = Ae^{\eta x}$ $\quad \eta^2 = -\frac{2mE}{\hbar^2}$

Inside well

- $-\frac{L}{2} < x < \frac{L}{2}$

$$u(x) = B\cos(kx)$$

$$k^2 = \frac{2m}{\hbar^2}(E + V_0)$$

Outside Well wave function has form

$$\boxed{u(x) = \begin{cases} Ae^{\eta x} & x < -L/2 \\ Ae^{-\eta x} & x > L/2 \end{cases} \qquad \eta > 0}$$

Inside well: potential constant, $E - V(x) = E - V_0 > 0 \Rightarrow$ solution is complex exponential

Parity forces

$$\boxed{u(x) = B\cos(kx) \qquad |x| < \frac{L}{2} \qquad k > 0}$$

The relations of η, k to E and V_0 are

$$E = -\frac{\hbar^2}{2m}\eta^2 \equiv \frac{\hbar^2}{2m}k^2 - V_0$$

Imposing continuity

1) continuity of $u(x)$ at $x = L/2$

$$\left.\lim_{x \nearrow \frac{L}{2}} u(x) = B\cos\left(\frac{kL}{2}\right)\ \right\} = \text{impose equality}$$

$$\lim_{x \searrow \frac{L}{2}} u(x) = Ae^{-\eta L/2}$$

Hence $\quad B\cos\left(k\frac{L}{2}\right) = Ae^{-\eta L/2}$

2) continuity of $u'(x)$ at $x = L/2$

$$\lim_{x \nearrow \frac{L}{2}} u'(x) = Bk\cos\left(\frac{kL}{2}\right) \qquad \lim_{x \searrow \frac{L}{2}} u'(x) = -\eta Ae^{-\eta\frac{L}{2}}$$

Solving 1) fixing

$$B = \frac{A}{\cos\left(\frac{kL}{2}\right)} e^{-\eta L/2}$$

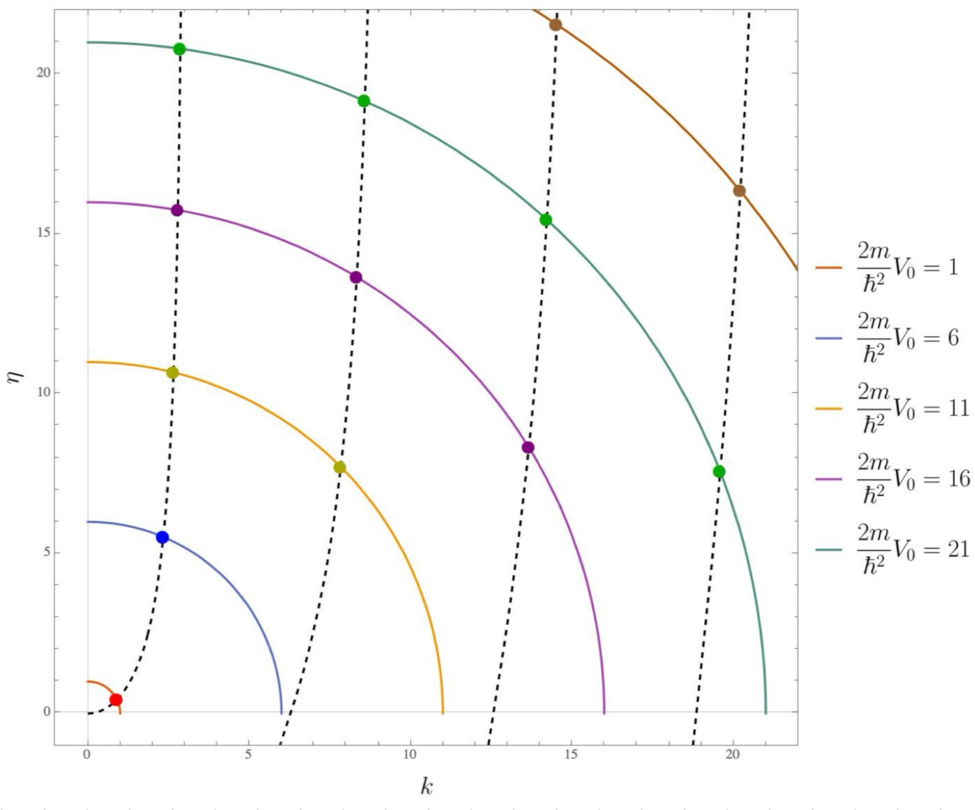
We get $\quad \eta \frac{\cancel{B}\cos(kL/2)}{\cancel{e^{-\eta L/2}}} \cancel{e^{-\eta L/2}} = \cancel{B} k\sin\left(\frac{kL}{2}\right)$

$$\Longrightarrow \quad \eta\cos\left(\frac{kL}{2}\right) = k\sin\left(\frac{kL}{2}\right)$$

$$\Longrightarrow \quad \boxed{k\tan\left(\frac{kL}{2}\right) = \eta} \qquad \boxed{\eta^2 + k^2 = \frac{2m}{\hbar^2} V_0} \quad \text{equation of circle}$$

dashed lines

Solutions are intersections of the 2 plots in (k, η) plane



spectrum $\{E\}$ is discrete

limited (not ∞)

Looking at limit of infinitely deep well $V_0 \to \infty$. In order to satisfy

$$\eta^2 + k^2 = \frac{2m}{\hbar^2} V_0$$

take $\eta \to \infty$ in concert. At the same time, transcendental equation is satisfied for

$$kL \to (2n-1)\pi \qquad n \in \mathbb{N}$$

Now clearly energy $E \propto -\eta^2$ diverges to ∞.

We always have freedom to choose reference from which we measure energies of the system. In this limit we choose reference to be the floor of the potential $-V_0$.

Redefine energy $E' = E + V_0$. Then

$$E' = \frac{\hbar}{2m}k^2 = \frac{\hbar^2 \pi}{2mL^2}(2n-1)^2$$

which is the odd part of energy of particle of the box.

Odd case

Works out like the even case. Solution has form

$$u(x) = \begin{cases} Ae^{\eta x} & x < -L/2 \\ B\sin(kx) & -L/2 < x < L/2 \\ -Ae^{-\eta x} & x > L/2 \end{cases}$$

since $u(-x) = -u(x)$

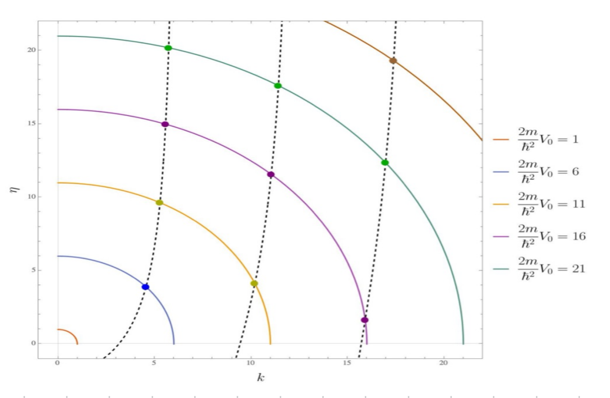
Imposing continuity

continuity of $u(x)$: $B\sin\left(k\frac{L}{2}\right) = Ae^{-\eta L/2}$

continuity of $u'(x)$: $kB\cos\left(k\frac{L}{2}\right) = -\eta A e^{-\eta L/2}$

we get equations

$$\boxed{\frac{k}{\tan(k\frac{L}{2})} = -\eta} \qquad \boxed{\eta^2 + k^2 = \frac{2m}{\hbar^2}V_0}$$



We are no longer guarunteed to have atleast one solution.

The first dashed line emerges from the $k=0$ axis into the first quadrant at $kL = \pi$.

The circle intersects this line only if

$$\frac{2mV_0}{\hbar^2} > \frac{\pi^2}{L^2} \implies \frac{L^2 m V_0}{\hbar^2} > \frac{\pi^2}{2}$$

Throwing particles at walls

Turn to study scattering states.

We throw particles at a potential wall and see what happens.

$$u(x) \underset{|x|\to\infty}{\sim} a e^{ikx} \quad \text{not integrable}$$

Consider wavefunctions of form

$$u_k(x) = A_k e^{ikx} \qquad k\in\mathbb{R}, \; A_k \in \mathbb{C}$$

with definite momentum $p=\hbar k$, but not admissible since it is not normalizable.

Therefore instead of associating wavefunctions to single particles, we take them to be describing a continuous beam of particles.

$$P(x,t) = |\psi(x,t)|^2 = |u_k(x) e^{\frac{-iEt}{\hbar}}|^2$$
$$= |A|^2$$

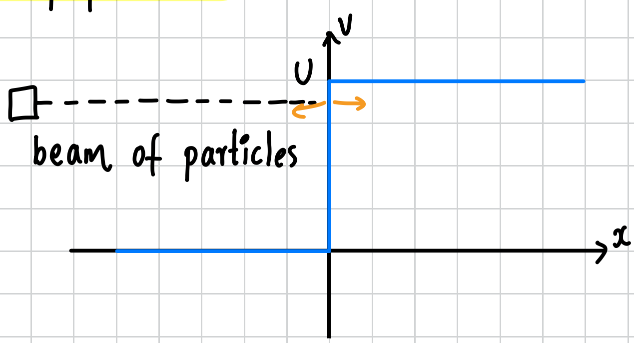
$|A|^2$: Average density of particles

Computing probability current

$$J(x) = \frac{i\hbar}{2m}\left[\bar{\psi}(x,t)\frac{\partial}{\partial x}\psi(x,t) - \psi(x,t)\frac{\partial}{\partial x}\bar{\psi}(x,t)\right]$$
$$= |A|^2 \frac{p}{m}$$

which is average density $|A|^2$ x velocity p/m = average flux of particles

Step potential



$$V(x) = \begin{cases} 0 & x<0 \\ U & x>0 \end{cases}$$

$$-\frac{\hbar^2}{2m}u''(x) = (E - V(x))u(x)$$

• $x<0$, $V=0$

$$\boxed{u = Ae^{ikx} + Be^{-ikx} \qquad k = \frac{\sqrt{2mE}}{\hbar} > 0}$$

Here Ae^{ikx} is the right moving part.

- $x>0$, the potential is non-zero but constant $\Rightarrow$ we get exponentials

$$u(x) = Ce^{ik'x} + De^{-ik'x} \qquad k' = \frac{\sqrt{2m(E-U)}}{\hbar}$$

$k' \in \mathbb{R}$ for $E>U$

This is too general.

$k' \in \mathbb{C}$ for $E<U$ imaginary

- For $E<U$,

$$-ik' = \eta' \quad \text{with} \quad \eta' = \frac{\sqrt{2m(U-E)}}{\hbar} > 0$$

Then

$$u(x) = Ce^{-\eta' x} + De^{\eta' x}$$

not normalizable $\Longrightarrow$ therefore set $D=0$

- For $E>U$, De^{-ikx} represents left moving wave, but left moving should only exist for $x<0$. no emitter at $x>0$ going left $\Rightarrow D=0$

Therefore the solution looks like

$$u(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x<0 \\ Ce^{ik'x} & x>0 \end{cases}$$

Imposing continuity,

1) Continuity of $u(x)$: $A+B=C$

2) Continuity of $u'(x)$: $ik(A-B) = ik'C$

The solutions are

$$B = \frac{k-k'}{k+k'}A \qquad C = \frac{2k}{k+k'}A$$

c.f with reflection and transmission amplitudes for waves

Calculating fluxes,

$$J_{inc} = |A|^2 \frac{\hbar k}{m}$$

$$J_{refl} = |B|^2 \frac{\hbar k}{m} = |A|^2 \frac{\hbar k}{m}\left(\frac{k-k'}{k+k'}\right)^2$$

$$J_{trans} = |C|^2 \frac{\hbar k'}{m} = |A|^2 \frac{\hbar k'}{m} \frac{4k^2}{(k+k')^2}$$

Calculating the ratio of fluxes,

$$\boxed{\begin{array}{l} \text{reflection coefficient}: \quad R \doteq \dfrac{J_{refl}}{J_{inc}} = \left(\dfrac{k-k'}{k+k'}\right)^2 \\[2em] \text{transmission coefficient}: \quad T \doteq \dfrac{J_{trans}}{J_{inc}} = \dfrac{4kk'}{(k+k')^2} \end{array}}$$

Note: $R+T=1$

Looking at limiting case

- $E \longrightarrow U$: In this limit, $k' \longrightarrow 0$ and $(R,T) \longrightarrow (1,0)$, so when the particle has barely enough energy to make it over the well, it is simply reflected back with almost 100% chance

- $E \longrightarrow \infty$: Now $k' \approx k$ and $(R,T) \rightarrow (0,1)$

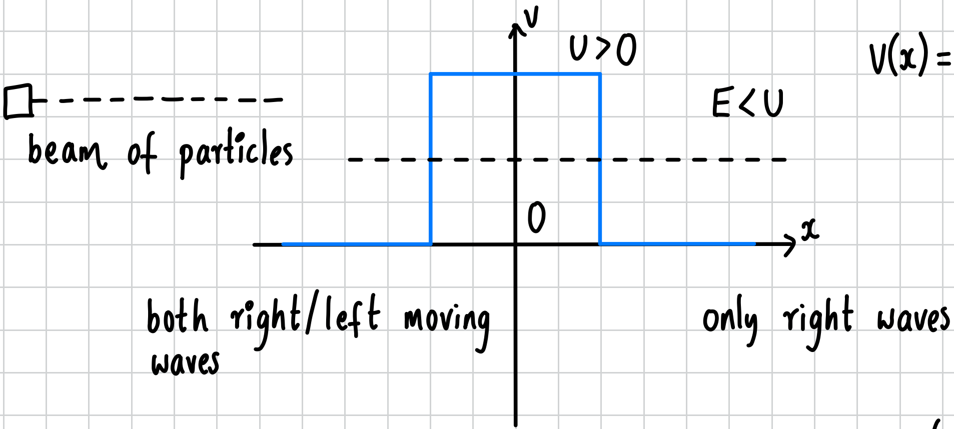
  Energy grows more and more, there is less and less probability that the particle is reflected back.

When $E < U$, in the region $x>0$ region is

$$u(x) = Ce^{-\eta' x} \qquad \eta' = \frac{2m(U-E)}{\hbar} > 0$$

Tunnelling

Consider a bump potential.



$$V(x) = \begin{cases} U & -L/2 < x < L/2 \\ 0 & \text{otherwise} \end{cases}$$

$u(x) = e^{ikx}$ is right moving

$\psi(x,t) = e^{i(kx - \frac{E}{\hbar}t)}$ $\quad k>0$

Interested in situations $0 < E < U$

Our solution has form, $B, C, D, F \in \mathbb{C}$

$$u(x) = \begin{cases} e^{ikx} + Be^{-ikx} & x < -L/2 \\ Ce^{-\eta x} + De^{\eta x} & |x| < L/2 \\ Fe^{ikx} & x > L/2 \end{cases} \qquad \begin{cases} k = \frac{\sqrt{2mE}}{\hbar} > 0 \\ \eta = \frac{\sqrt{2m(E-U)}}{\hbar} > 0 \end{cases}$$

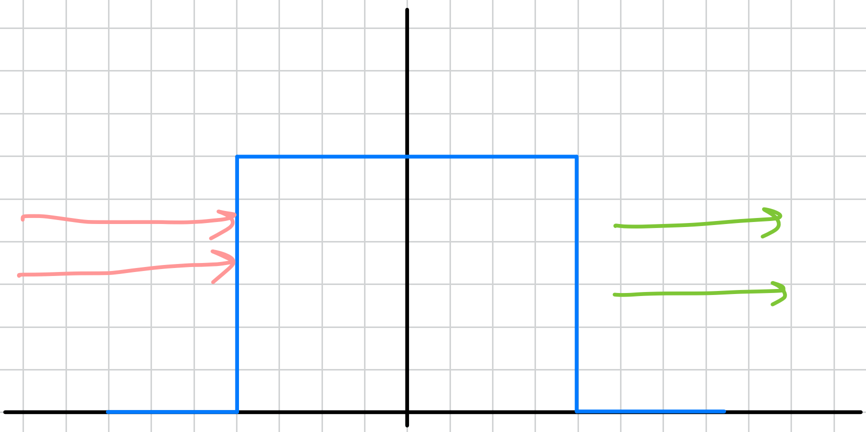
Imposing continuity:

1) Continuity of $u(x)$ at $x = -\frac{L}{2}$: $e^{ik\frac{L}{2}} + Be^{ik\frac{L}{2}} = Ce^{\eta\frac{L}{2}} + D$ eq 1

2) Continuity of $u'(x)$ at $x = -\frac{L}{2}$: $ik(e^{-ik\frac{L}{2}} - Be^{ikL/2}) = \eta(De^{-\eta\frac{L}{2}} - Ce^{\eta\frac{L}{2}})$ eq 2

3) Continuity of $u(x)$ at $x = \frac{L}{2}$: $Fe^{ik\frac{L}{2}} = Ce^{-\eta\frac{L}{2}} + De^{\eta\frac{L}{2}}$ eq 3

4) Continuity of $u'(x)$ at $x = \frac{L}{2}$: $ikFe^{ik\frac{L}{2}} = \eta(De^{\eta L/2} - Ce^{-\eta L/2})$ eq 4



Incoming flux

$$J_{inc}(x) = \frac{-i\hbar}{2m}\left[u(x)\partial_x u(x) - u\partial_x \bar{u}(x)\right]$$

$$= \frac{-i\hbar}{2m}\left[\left(e^{-ikx}+\bar{B}e^{+ikx}\right)\left(ike^{+ikx}-ikBe^{-ikx}\right)-\left(e^{ikx}+Be^{-ikx}\right)\left(-ie^{-ikx}+ik\bar{B}e^{ikx}\right)\right]$$

$$= \frac{-i\hbar}{2m}\left[ik\left(1-|B|^2-Be^{2ikx}+\bar{B}e^{+2ikx}\right)--ik\left(1-|B|^2-\bar{B}e^{+2ikx}+Be^{-2ikx}\right)\right]$$

$$= \frac{\hbar k}{m}\left(1-|B|^2\right)$$

Transmitted flux

Similarly

$$J_{trans} = \frac{\hbar k}{m}|F|^2$$

From continuity equations, consider the following sum

$$k(\text{eq } 1) - i(\text{eq } 2) + (k\cosh(\eta L) + i\eta\sinh(\eta L))(\text{eq } 3) - \frac{k\sinh(\eta L) + i\eta\cosh(\eta L)}{\eta}(\text{eq } 4)$$

$$\Longrightarrow \boxed{F = \frac{2k\eta e^{-ikL}}{2k\eta\cosh(\eta L) - i(k^2-\eta^2)\sinh(\eta L)}}$$

Then the transmission probability reads

$$T = |F|^2 = \frac{4k^2\eta^2}{4k^2\eta^2\cosh^2(\eta L) + (k^2-\eta^2)\sinh^2(kL)} = \frac{1}{1 + \frac{(k^2+\eta^2)^2}{4k^2\eta^2}\sinh^2(L\eta)}$$

So there is a non-zero chance that the particle makes it through the potential wall

↳ "quantum tunnelling"

Looking at limiting case: when energy of particle is very low

$\Longrightarrow$ $U-E$ very large compared to a feature of the system with dimension $\underset{\text{energy}}{[E]}$

By dimensional analysis, this quantity is $\hbar/mL^2$. Hence

$$U - E \gg \frac{\hbar^2}{mL^2} \Longrightarrow \eta L \gg 1$$

So the regime can be reached in many ways, either taking U much larger than E or L being very large or $\hbar$ being very small (classical limit). They are the same regime.

Eigenvalue Problem of Sturm-Liouville type

We will look at a more general and formal look at the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}u''(x) + V(x)u(x) = E\,u(x)$$

and more generally, at a special case of equations that this belongs to: Sturm-Liouville problems

SPECTRAL PROBLEMS

The time-independent Schrödinger equation is a special case of a second order linear ODE, whose general form is

$$(L\cdot u)(x) \doteq u''(x) + p(x)u'(x) + q(x)u(x) = \lambda \rho(x)u(x)$$

differential operator

$u : \mathbb{R} \longrightarrow \mathbb{C} \qquad u \in C^2[a,b]$

$p(x), q(x), \rho(x)$ are complex valued functions,

$\lambda \in \mathbb{C}$: the spectral parameter

We need boundary conditions (Dirichlet, Neumann, etc)

$$\begin{cases} u''(x) + p(x)u'(x) + q(x)u(x) = \lambda\rho(x)u(x) & \forall x \in (a,b) \\ B_L(u(x), u'(x)) = 0 \\ B_R(u(x), u'(x)) = 0 \end{cases}$$

B_a and B_b are left and right boundary conditions.

The spectral problems for operator L:

Find all the eigenvalues λ that satisfy boundary condition,

$B_a(u,u') = 0 \qquad B_b(u,u') = 0$

$x = a \qquad x = b$

Some terminology:

- $\lambda \in \mathbb{C}$: eigenvalue
- $u(x)$: eigenfunction associated to some eigenvalue λ
- $\{\lambda_m\}_{m \subset I \subseteq \mathbb{N}}$ is the set of all eigenvalues.

Note: Since Sturm-Liouville problem is linear, if $u(x)$ and $v(x)$ are 2 solutions,

$$\alpha u(x) + \beta v(x) \qquad \forall \alpha, \beta \in \mathbb{C}$$

is a solution.

Sturm-Liouville problems (S-L problems)

A special case of spectral problem

$$\begin{cases} (L\cdot u)(x) \doteq -\dfrac{1}{\rho(x)}\dfrac{d}{dx}\left(P(x)u'(x)\right) + \dfrac{Q(x)}{\rho(x)}u(x) = \lambda u(x) & \forall\, x\in(a,b)\subseteq\mathbb{R} \\ B_a(u,u') = 0 \\ B_b'(u,u') = 0 \end{cases}$$

Sturm-Liouville problem

where B_a and B_b' satisfy

$$\forall\, u,v\in C^1 \qquad \left[\bar{v}'(x)\,P(x)u(x) - \bar{v}(x)\,P(x)u'(x)\right]_{x=a}^{x=b} = 0$$

$u(x)$ is complex
$\rho(x)>0$ is real valued
$P(x)$, $Q(x)$ is real valued

Aside:

- vector inner product $\langle \underline{v}, \underline{w}\rangle$
- M is hermitian if $\langle \underline{v}, M\underline{w}\rangle = \langle M^{\dagger}\underline{v}, \underline{w}\rangle$, $M\in Mat(\mathbb{C})$

We need this condition because

$$I = \int_a^b dx\, \rho(x)\,\bar{v}(x)(L\cdot u)(x) = \int_a^b dx\, \bar{v}(x)\left[-\frac{d}{dx}\left(P(x)u'(x)\right) + Q(x)\,u(x)\right]$$

integration by parts

$$= \left[-\bar{v}(x)u'(x)\,P(x)\right]_{x=a}^{x=b} + \int_a^b dx\left[P(x)u'(x)\bar{v}'(x) + Q(x)\,u(x)\,\bar{v}(x)\right]$$

$$= \left[\bar{v}'(x)u(x)\,P(x) - \bar{v}(x)\,u'(x)\,P(x)\right]_{x=a}^{x=b} + \int_a^b dx\, u(x)\left[-\frac{d}{dx}\left(P(x)\,\bar{v}'(x)\right) + Q(x)\,\bar{v}(x)\right]$$

$$= \left[\bar{v}'(x)u(x)\,P(x) - \bar{v}(x)\,u'(x)\,P(x)\right]_{x=a}^{x=b} + \int_a^b dx\, u(x)\overline{\left[-\frac{d}{dx}\left(P(x)\,v'(x)\right) + Q(x)\,v(x)\right]}$$

$$= \underbrace{\left[\bar{v}'(x)u(x)\,P(x) - \bar{v}(x)\,u'(x)\,P(x)\right]_{x=a}^{x=b}}_{0 \text{ for S-L problem}} + \int_a^b dx\, \rho(x)\,\overline{(L\cdot v)}(x)\,u(x)$$

$$\Longrightarrow \boxed{\int_a^b dx\,\rho(x)\,\bar{v}(x)(L\cdot u)(x) = \int_a^b dx\,\rho(x)\,\overline{(L\cdot v)}(x)\,u(x)}$$

Operator L is Hermitian

Define inner product for complex functions on $[a,b]$

$$\boxed{\langle v, u\rangle_\rho = \int_a^b dx\, \rho(x)\bar{v}(x)u(x)}$$

Inner product

Properties

1) $\langle v, \alpha u_1 + \beta u_2\rangle = \alpha\langle v, u_1\rangle + \beta\langle v, u_2\rangle \quad \forall \alpha, \beta \in \mathbb{C}$
2) $\overline{\langle v, u\rangle} = \langle u, v\rangle$
3) $\langle u, u\rangle \geq 0$
4) $\langle u, u\rangle = 0 \iff u(x) \equiv 0$

In this notation

$$\boxed{\langle v, L\cdot u\rangle = \langle L\cdot v, u\rangle}$$

Hermitian

In relation to quantum mechanics, TDSE is an S-L problem

$$-\frac{\hbar^2}{2m}u''(x) + V(x)u(x) = Eu(x)$$

$$\rho(x) = 1 \qquad P(x) = +\frac{\hbar^2}{2m} \qquad Q(x) = V(x) \quad \lambda = E$$

Verifying that S-L problem satisfies D-D and N-N conditions

- D-D:
  Suppose boundary conditions are $B_a(u,u') = u(a)$, $B_b(u,u') = u(b)$

  $$\text{D-D} \Longrightarrow u(a) = 0 \text{ and } u(b) = 0$$
  $$\Longrightarrow \left[\bar{v}'(x)u(x)P(x) - \bar{v}(x)u'(x)P(x)\right]_{x=a}^{x=b} \equiv 0$$

- N-N:
  Suppose boundary conditions are $B_a(u,u') = u'(a)$, $B_b(u,u') = u'(b)$

  $$\text{N-N} \Longrightarrow u'(a) = 0 \text{ and } u'(b) = 0$$
  $$\Longrightarrow \left[\bar{v}'(x)u(x)P(x) - \bar{v}(x)u'(x)P(x)\right]_{x=a}^{x=b} \equiv 0$$

The wavefunction is

$$\psi(x,t) = u(x)\, e^{-iE/\hbar\, t}$$

$$J(x) = \frac{-i\hbar}{2m}\left[\bar{\psi}(x,t)\frac{d}{dx}\psi(x,t) - \psi(x,t)\frac{d}{dx}\bar{\psi}(x,t)\right]$$

$$= -\frac{i\hbar}{2m}\left[\bar{u}(x)u'(x) - \bar{u}'(x)u(x)\right]$$

$$= +i\left[\bar{u}'(x)P(x)u(x) - \bar{u}(x)P(x)u(x)\right] = J(x) \Rightarrow J(a) - J(b) = 0$$

if S-L boundary conditions are true,

$$\Downarrow$$

$$\frac{dP_{[a,b]}}{dt} = 0$$

where

$$P_{[a,b]} = \int_a^b dx\,|\psi(x,t)|^2 = P(a) - P(b)$$

PROPERTIES OF STURM-LIOUVILLE PROBLEM

Two functions are **orthogonal** iff

$$\langle v,u\rangle_\rho = \int_a^b dx\,\rho(x)\bar{v}(x)u(x) = 0$$

Recall integral

$$\frac{2}{\pi}\int_0^\pi \sin(nx)\sin(mx) = \delta_{mn} \quad m,n\in\mathbb{Z}$$

$$\left\{ u_n(x) = \sqrt{\frac{2}{\pi}}\sin(nx) \right\} \quad n\in\mathbb{Z}$$

↳ orthogonal normalized functions

Theorem Reality of the spectrum for Sturm-Liouville problems

The spectrum $\{\lambda_m\}_{m\subset I\mathbb{Z}}$ of a Sturm-Liouville problems are real $\lambda_m\in\mathbb{R}$, $m\in I$

Proof:

Start with S-L problem

$$(L\cdot u)(x) = \lambda u(x)$$

with $\lambda\in\mathbb{C}$ and $u(x)\equiv 0$.

Then we compute

$$\lambda\langle u,u\rangle > 0 \implies \langle u, L\cdot u\rangle = \langle L\cdot u, u\rangle = \langle \lambda u, u\rangle = \overline{\langle u, \lambda u\rangle} = \overline{\lambda}\,\overline{\langle u,u\rangle}$$

$$= \overline{\lambda}\langle u,u\rangle$$

$$\implies (\lambda - \overline{\lambda})\langle u,u\rangle = 0$$

$$\implies \lambda - \overline{\lambda} = 0 \qquad \text{since } \langle u,u\rangle \neq 0$$

$$\implies \lambda = \overline{\lambda}$$

$$\implies \lambda \in \mathbb{R}$$

■

Theorem Orthogonality of eigenfunctions in Sturm-Liouville problems

Let $u_1(x)$ and $u_2(x)$ be eigenfunctions (solutions) of a Sturm-Liouville type operator L associated to different eigenvalues λ_1 and λ_2. Then

$$\langle u_1, u_2\rangle = 0$$

Proof: $\lambda_2\langle u_1,u_2\rangle = \langle u_1, L\cdot u_2\rangle$

$$= \langle L\cdot u_1, u_2\rangle$$

$$= \overline{\lambda}_1\langle u_1,u_2\rangle$$

$$\implies (\lambda_2 - \overline{\lambda}_1)\langle u_1,u_2\rangle = 0 \qquad \lambda_1 \neq \lambda_2$$

$$\implies \langle u_1,u_2\rangle = 0$$

■

Reduction of spectral problems to Sturm-Liouville type

Any second order ODE can be brought to S-L problem

Consider general case

$$u''(x) + p(x)u'(x) + q(x)u(x) = \lambda w(x)u(x)$$

Multiplying both sides by $R(x)$

$$R(x)u''(x) + R(x)p(x)u'(x) + R(x)q(x)u(x) = R(x)\lambda w(x)u(x)$$

Need to recast it into S-L form

$$-\frac{d}{dx}\left(P(x)u'(x)\right) + Q(x)u(x) \equiv -P(x)u''(x) - P'(x)u'(x) + Q(x)u(x) = \lambda\rho(x)u(x)$$

Therefore we get

$$R(x) = -P(x) \qquad \text{and} \qquad R(x)p(x) = -P'(x)$$

$$\Longrightarrow \frac{P'(x)}{P(x)} = p(x) \Longrightarrow P(x) = \exp\left[\int_0^x ds\, p(s)\right]$$

Therefore, we have

$$\boxed{\begin{aligned} P(x) &= \exp\left[\int_0^x ds\, p(s)\right] \\ Q(x) &= -q(x)\exp\left[\int_0^x ds\, p(s)\right] \\ \rho(x) &= -w(x)\exp\left[\int_0^x ds\, p(s)\right] \end{aligned}}$$

Example:

$$x^2 u''(x) - 2x u'(x) + u(x) = -\lambda x^4 u(x)$$

$$\Longrightarrow u''(x) - \frac{2}{x} u'(x) + \frac{1}{x^2} u(x) = -\lambda x^2 u(x)$$

Coefficients are

$$p(x) = -\frac{2}{x}, \quad q(x) = \frac{1}{x^2} \qquad w(x) = -x^2$$

The primitive of $p(x)$

$$\int_1^x p(s)\, ds = \int_1^x -2\frac{dx}{x} = -2\log x$$

Now by substitution

$$P(x) = x^{-2}$$

$$Q(x) = -\frac{1}{x^2} x^{-2} = -x^{-4}$$

$$\rho(x) = -(-x^2)(cx^{-2}) = 1$$

Hence the Sturm-Liouville form of the equation is

$$-\frac{d}{dx}\left(\frac{1}{x^2} u'(x)\right) - \frac{u(x)}{x^4} = \lambda u(x)$$

Quantum Mechanical interpretation of S-L boundary conditions

Consider

$$\psi(x,t) = u(x) e^{-i\frac{E}{\hbar}t}$$

with the function $u(x)$ satisfying S-L type ODE

$$-(P(x)u'(x)) + Q(x)u(x) = \lambda \rho(x) u(x) \,, \qquad \begin{cases} P(x) = \hbar/2m \\ Q(x) = V(x) \\ \rho(x) = 1 \\ \lambda = E \end{cases}$$

From the definition of probability current

$$J(x,t) = \frac{-i\hbar}{2m}\left(\bar{\psi}(x,t)\frac{d}{dx}\psi(x,t) - \psi(x,t)\frac{d}{dx}\bar{\psi}(x,t)\right)$$

Substituting wave eqn

$$J(x,t) \equiv J(x) = \frac{i}{\hbar}\left(\bar{u}'(x)\frac{\hbar^2}{2m}u(x) - \bar{u}(x)\frac{\hbar}{2m}u'(x)\right)$$

$$= \frac{i}{\hbar}\left(\bar{u}'(x)P(x)u(x) - \bar{u}(x)P(x)u'(x)\right)$$

The S-L condition reads

$$\left[\bar{v}'(x)P(x)u(x) - \bar{v}(x)P(x)u'(x)\right]_{x=a}^{x=b} = 0$$

$$\Longrightarrow J(b) - J(a) = 0$$

Recall by conservation of probability

$$\frac{\partial}{\partial t}P(x,t) + \frac{d}{dx}J(x) = 0$$

$$P_{[a,b]}(t) = \int_a^b dx\, P(x,t)$$

$$\frac{d}{dt}P_{[a,b]}(t) = \int_a^b dx \frac{\partial}{\partial x}P(x,t) = -\int_a^b dx\frac{d}{dx}J(x) = J(b) - J(a) = 0$$

Regular S-L problems

Eigenfunctions of S-L problems have orthogonality relation. We want to know if they can be used to reconstruct any function in defining interval $[a,b]$

(like Fourier series)

In mathematical Jargon

"Do the set of eigenfunctions form a complete orthonormal system"

S-L problems produce complete orthonormal system under following conditions

- a, b are finite
- $P(x), P'(x), Q(x), \rho(x)$ are real and continuous in $[a,b]$
- $P(x), \rho(x)$ are strictly positive in $[a,b]$

Theorem

$\forall$ regular S-L problems, the following are true

1) The eigenvalues are ∞ many, countable, form an increasing sequence

$$\{\lambda_m\}_{m\in\mathbb{N}} \qquad \lambda_1 \leq \lambda_2 \leq \lambda_3 \cdots\cdots$$

with limiting behaviour

$$\lim_{m\to\infty} \lambda_m = \infty$$

2) To each λ_m, is associated a unique eigenfunction (up to multiplication by constant)

$$u_m(x)$$

that has exactly $m-1$ zeroes in $x\in[a,b]$

3) The set of normalized eigenfunctions is a complete orthonormal system

$$\{u_m(x)\}_{m\in\mathbb{N}}$$

Power Series Method

HARMONIC OSSCILATOR

Harmonic oscillator has potential

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

which gives the quantum harmonic oscillator

$$\boxed{-\frac{\hbar^2}{2m}u''(x) + \frac{1}{2}m\omega^2 x^2 u(x) = Eu(x)}$$

Quantum Harmonic Oscillator

Taylor Series and Analytic functions

Let $f \in C^\infty(\mathbb{R})$. Select x_0

$$\boxed{\sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x_0)(x-x_0)^n = P(x)}$$

Taylor expansion

Definition Analytic function

If for any interval I such that $x_0 \in I$,

if $\forall x \in I$, $P(x) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x_0)(x-x_0)^n$ converges on I

$\Longrightarrow f$ is analytic on I

Example:

- $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$
- $\cos(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n}$

$\forall x \in (-\infty, \infty) = \mathbb{R}$

- $\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1}$
- $\sinh(x) = \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} x^{2n+1}$
- $\cosh(x) = \sum_{n=0}^{\infty} \frac{1}{(2n)!} x^{2n}$

Functions can be analytic on other intervals.

Example

- $\log(1+x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n} x^n \qquad x \in (-1, 1]$
- $\log(1-x) = \sum_{n=0}^{\infty} \frac{x^n}{n} \qquad x \in [-1, 1)$
- $(1+x)^\alpha = \sum_{n=0}^{\infty} \binom{\alpha}{n} x^n \qquad x \in (-1, 1) \qquad \alpha \in (-1, 1)$

Properties: f, g analytic in an interval $I \subseteq \mathbb{R}$ about x

1) any sum of products of f and g are analytic (linear combination) on I
2) if $g(x_0) = 0$, $g(I') \not\ni 0$, $I' \subseteq I$

   if f analytic on interval $x_0 \in I$, then

$$\frac{f(x)}{g(x)} \text{ is analytic in } I' \subseteq I \text{ about } I$$

3) all derivatives of analytic functions are analytic

Ratio test

Theorem Suppose $(a_j)_{j \in \mathbb{N}}$ is a sequence of non-zero terms, such that

$$\left| \frac{a_{j+1}}{a_j} \right| \longrightarrow r \quad \text{as } j \longrightarrow \infty$$

Then

$$\sum_{j=1}^{\infty} a_j \begin{cases} \text{converges} & r<1 \\ \text{diverges} & r>1 \\ \text{non-conclusive} & r=1 \end{cases}$$

Finding radius of convergence of power series

$$\sum_{n=0}^{\infty} a_n (x-x_0)^n = P(x)$$

Applying ratio test

$$\left| \frac{a_{n+1}(x-x_0)^{n+1}}{a_n (x-x_0)^n} \right| = \left| \frac{a_{n+1}}{a_n} (x-x_0) \right|$$

if convergent

$$\left|\frac{a_{m+1}(x-x_0)}{a_m}\right| \longrightarrow \frac{1}{R}|x-x_0| < 1 \quad \text{as } n \to \infty$$

$$\Longrightarrow \quad |x-x_0| < R$$

R: radius of convergence

Therefore $P(x)$ converges in interval (x_0-R, x_0+R)

if $\left|\frac{a_{m+1}}{a_m}(x-x_0)\right| \longrightarrow 0 < 1$ for all $n \Longrightarrow R = \infty$

Equivalent formulation

Consider a series

$$\sum_{n=0}^{\infty} a_n (x-x_0)^n$$

Then

$$\boxed{\lim_{n\to\infty}\left|\frac{a_n}{a_{n+1}}\right| = R \text{ or } \infty}$$

R: radius of convergence, interval (x_0-R, x_0+R)

if $R=\infty \Longrightarrow \mathbb{R} = (-\infty, \infty)$

Example

1) $f(x) = e^x = \sum_{m=0}^{\infty} \frac{1}{m!} x^m$; $\left|\frac{a_{m+1}x}{a_m}\right| = \frac{(m)!\,x}{(m+1)!} \longrightarrow 0 < 1$ as $m \to \infty \quad \forall x$

$\Longrightarrow$ radius of convergence : $\mathbb{R} = (-\infty, \infty)$

2) $f(x) = \sum_{n=0}^{\infty} x^n$

$$\lim_{n\to\infty}\left|\frac{a_n}{a_{n+1}}\right| = \lim_{n\to\infty}|1| = 1 \Longrightarrow R = 1$$

Differentiating power series

$$\boxed{\frac{d^m}{dx^m}\sum_{m=0}^{\infty} a_m (x-x_0)^m = \sum_{m=1}^{\infty} a_m \frac{d^m}{dx^m}(x-x_0)^m}$$

Reduction of Harmonic Oscillator

$$u''(x) - x^2\frac{m^2\omega^2}{\hbar^2}u(x) = -\frac{2mE}{\hbar^2}u(x)$$

Dimensional Analysis

Note: $[E] = [V] = \frac{ML^2}{T^2}$

So

$$[E] = [V] = [m\omega^2x^2/2] = [m][\omega]^2[x]^2$$

$$\Longrightarrow \cancel{M}[\omega]^2\cancel{L^2} = \frac{\cancel{M}\cancel{L^2}}{T^2}$$

$$\Longrightarrow \boxed{[\omega] = \frac{1}{T}}$$

Further $[\hbar] = [E]T = \frac{ML^2}{T}$, we see

$$\left[\frac{m\omega}{\hbar}\right] = \frac{M/T}{ML^2/T} = L^{-2}$$

$$\left[\frac{mE}{\hbar^2}\right] = \frac{M}{[E]T^2} = \frac{M}{ML^2} = L^{-2}$$

Non-Dimensionalisation

Define

$$z = \sqrt{\frac{m\omega}{\hbar}}\,x \qquad \varepsilon = \frac{2mE}{\hbar^2}\frac{\hbar}{m\omega} = \frac{2E}{\hbar\omega}$$

$$v(z) \doteq u(x(z))$$

Substituting

$$\boxed{v''(z) + (\varepsilon - z^2)v(z) = 0}$$ Dimensionless Schrödinger Equation

For $\varepsilon = 1$: satisfied by Gaussian function

$$g(z) = e^{-z^2/2} \quad , \; g' = -zg$$

$$\frac{d^2}{dz^2}\left(e^{-z^2/2}\right) = (z^2-1)\,e^{-z^2/2}$$

For other other other potential solutions, see what happens for $|z| \to \infty$ (large $|z|$)

In this case ε negligible compared to z^2 $\Longrightarrow$ all solutions should behave as $e^{-z^2/2}$ for large z

Therefore define

$$h(z) = \frac{v(z)}{g(z)} = \frac{v(z)}{e^{-z^2/2}}$$

substituting into $v'' + (\varepsilon - z^2)v = 0$

$$\downarrow$$

$$\boxed{h''(z) - 2zh' + (\varepsilon - 1)h = 0}$$

$g(z) = e^{-z^2/2} \Rightarrow g' = -zg$

$\Rightarrow g'' = -g + z^2 g$

For large z, $g = e^{-z^2/2} \approx 0$

$\Rightarrow g'' \approx +z^2 g$

Hence in dimensionless eqn, ε neglected

$v'' \approx z^2 g''$ and g satisfies the equation

Power Series solution and energy spectrum

Strategy: Search for a solution in form of power series about $z = 0$

$$h(z) = \sum_{n=0}^{\infty} h_n z^n$$

Consider general ODE

$$u''(z) + p(z)u'(z) + q(z)u(z) = 0 \quad (*)$$

We say $z = z_0$ is

- z_0 is an ordinary point if $p(z)$ and $q(z)$ are analytic at z_0
- singular point if $(z - z_0)p(z)$ and $(z - z_0)^2 q(z)$ are analytic
- z_0 is irregular if none of the above is true

Theorem Cauchy's Theorem

Let z_0 be an ordinary point of equation $(*)$

$$u''(z) + p(z)u'(z) + q(z)u(z) = 0$$

and $p(z)$ and $q(z)$ have Taylor series about z_0 with convergence radii R_p and R_q

Then $\exists$ 2 linearly independent solutions to $(*)$ $u_i(z)$, $i = 1, 2$ with power series expansion

$$u_i(z) = \sum_{n=0}^{\infty} u_{i,n} (z - z_0)^n$$

with radii of convergence $\min(R_p, R_q) = R \leq R_i$

In
$$h''(z) - 2zh' + (\varepsilon-1)h = 0$$

$p(z) = -2z$, $q(z) = \varepsilon - 1$, both have $R = \mathbb{R} \Longrightarrow$ has a taylor series convergent everywhere about $x=0$

Observe
$$h(z) = \sum_{n=0}^{\infty} h_n z^n \Longrightarrow h'(z) = \sum_{n=1}^{\infty} n h z^{n-1}$$
$$\Longrightarrow h''(z) = \sum_{n=2}^{\infty} n(n-1) h_n z^{n-2}$$

Substituting
$$\sum_{n=2}^{\infty} n(n-1) h_n z^{n-2} - 2\sum_{n=1}^{\infty} n h_n z^n + (\varepsilon-1)\sum_{n=0}^{\infty} h_n z^n = 0$$

Shifting summation index (change of index: $m = n-2 \Rightarrow m = n+2$)
$$\sum_{n=2}^{\infty} n(n-1) h_n z^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1) h_{n+2} z^n$$

we get
$$[2h_2 + (\varepsilon-1)h_0] + \sum_{n=1}^{\infty} \left[(n+2)(n+1)h_{n+2} + (\varepsilon - 2n - 1)h_n\right] z^n = 0$$

The above equation must hold for all $z \Longrightarrow$ we need to independently cancel all coefficients of z^n

This gives
$$\boxed{h_{n+2} = \frac{(2n+1-\varepsilon)}{(n+1)(n+2)} h_n} \qquad (*)$$

2 undetermined constants h_0, h_1

Note:

Eq $(*)$ has the property it connects
- even indexed coefficients to even indexed coefficients
- odd indexed coefficients to odd indexed coefficients

Therefore we have 2 independent solutions.

Further the relation is homogeneous, so has form
$$\boxed{h_{2n} = H_e(n) h_0 \qquad h_{2n+1} = H_o(n) h_1}$$

Therefore,

1) $h_0 \neq 0,\ h_1 = 0 \implies$ even solutions

$\implies h(z) = h(-z)$

2) $h_0 = 0,\ h_1 \neq 0 \implies$ odd solutions

$\implies h(z) = -h(-z)$

The radius of convergence is

$$R^2 = \lim_{n\to\infty} \left|\frac{h_n}{h_{n+1}}\right| \left|\frac{h_{n+1}}{h_{n+2}}\right| = \lim_{n\to\infty} \left|\frac{h_n}{h_{n+2}}\right| = \lim_{n\to\infty} \left|\frac{(n+1)(n+2)}{2n+1-\varepsilon}\right| \longrightarrow \infty$$

$\implies R = \infty$

$\implies h(z)$ analytic on $\mathbb{R}$

We have 2 cases:

1) $\exists N \in \mathbb{N}$ s.t $\forall n \geq N,\ h_n = 0 \implies h(z)$ truncates to a polynomial.

$\implies v(z)$ is still normalizable as as asymptotic behaviour is dominated by $e^{-z^2/2}$

$\exists N \in \mathbb{N}$ s.t $\forall n \geq N,\ h_n = 0 \implies \exists N$ s.t $2N+1 = \varepsilon = \frac{2E}{\hbar\omega}$

$$\implies \boxed{E = \hbar\omega\left(N + \frac{1}{2}\right)}$$

2) $h_n \neq 0,\ \forall n \in \mathbb{N} \cup \{0\}$

For large $|z|$, behavior of z might interfere with exponential decay

For large n; $n \gg \max(1, \varepsilon)$

$$h_{n+2} \approx \frac{2}{n} h_n$$

and this is bad, this is same behavior as e^{z^2}. Observe

$$e^{y^2} = \sum_{n=0}^{\infty} \frac{y^{2n}}{n!} \implies a_n = \begin{cases} \frac{1}{(n/2)!} & n \text{ even} \\ 0 & n \text{ odd} \end{cases}$$

$$ye^{y^2} = \sum_{n=0}^{\infty} \frac{y^{2n+1}}{n!} \implies a_n = \begin{cases} 0 & n \text{ even} \\ \frac{1}{\left(\frac{n-1}{2}\right)!} & n \text{ odd} \end{cases}$$

From the above 2 Taylor expansions, we get recurrence relation

$$a_{n+2} = \frac{2}{n} a_n$$

Therefore $h(z) \approx e^{z^2} \implies v(z) \xrightarrow[|z|\to\infty]{} e^{-z^2/2} e^{z^2} = e^{z^2/2}$

NOT normalizable

Therefore for $v(z)$ to be normalizable, $\{h_n\}_{n=1}^{\infty}$ must truncate, and we have

$$\boxed{E_N = \hbar\omega\left(N + \frac{1}{2}\right)}$$

Now

$$E_{N+1} - E_N = \hbar\omega \quad \text{energy equally placed}$$

The Wavefunctions: the solutions

Important!

$$\int_{\mathbb{R}} dx\, x^{2n} e^{-\frac{Ax^2}{2}} = \sqrt{\frac{\pi}{A}}\, A^{-n} \prod_{l=1}^{n} \left(l - \frac{1}{2}\right)$$

▶ $N = 0 \implies E = \frac{\hbar\omega}{2}$

degree of $h(z)$ is of degree $N=0 \implies h(z) = h_0$ constant

$$v(z) = h_0 e^{-z^2/2} \xrightarrow[\text{norm}]{} \boxed{u_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}}$$

▶ $N = 1 \implies E_0 = 3\hbar\omega/2$

degree of $h(z)$ is $N=1 \implies$ all $h_n = 0 \quad \forall\, n \geq 2$

$\implies h_0 = 0$ inorder to cancel all even terms.

Hence $h(z) = h_1 z$. Find h_1 by normalization

$$v_1(z) = h_1 z e^{-z^2/2} \xrightarrow[\text{norm}]{} \boxed{u_1(x) = \left(\frac{4m^3\omega^3}{\pi\hbar^3}\right)^{1/4} x e^{-\frac{m\omega}{2\hbar}x^2}}$$

▶ $N=2 \implies E_0 = 5\hbar\omega/2$

degree of $h(z)$ is $N=2 \implies$ all $h_n = 0 \quad \forall\, n \geq 3$

$\implies h_1 = 0$ to cancel odd terms

Hence $h(z) = h_0 + h_2 z^2$ and h_2 determined by recursion eqn above

$$h_2 = -2h_0$$

So we get wavefunction

$$v_2(z) = h_0(1-2z^2)e^{-z^2/2} \xrightarrow[\text{norm}]{} \boxed{u_2(x) = \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(1 - 2\frac{m\omega}{\hbar}x^2\right)e^{-\frac{m\omega}{2\hbar}x^2}}$$

▶ $N=3 \implies E_0 = 7\hbar\omega/2$

degree of $h(z)$ is $N=3 \implies$ all $h_n = 0 \quad \forall\, n \geq 4$

$\implies h_0 = 0$ to cancel even terms

Hence $h(z) = h_1 z + h_3 z^3$ and h_3 determined by recursion eqn above

$$h_3 = -\frac{2}{3}h_1$$

So we get wavefunction

$$v_3(z) = h_1 z\left(1 - \frac{2z^2}{3}\right)e^{-z^2/2} \xrightarrow[\text{norm}]{} \boxed{u_3(x) = \left(\frac{9m^3\omega^3}{\pi h^3}\right)^{1/4} x\left(1 - \frac{2}{3}\frac{m\omega}{\hbar}x^2\right)e^{-\frac{m\omega}{2\hbar}x^2}}$$

<u>Example calculations:</u>

1) $N=0 \implies \deg(h(z)) = 0$

$\implies h(z) = h_0$

Shown that $v(z) = h(z)e^{-z^2/2} \implies v_0(z) = h_0 e^{-z^2/2}$

Substituting $z = \sqrt{\frac{m\omega}{\hbar}}\,x \implies u_0(x) = h_0 e^{-\frac{m\omega}{2\hbar}x^2}$

Normalising

$$\int_{-\infty}^{\infty} u_0(x)\bar{u}_0(x)\,dx = \int_{-\infty}^{\infty} h_0^2 e^{-\frac{m\omega}{\hbar}x^2} = 1 \implies h_0^2\sqrt{\frac{\pi}{\frac{m\omega}{\hbar}}} = 1$$

$$\implies h_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}$$

2) $N=1 \Longrightarrow \deg(h(z))=1$ and $h_n = 0 \ \forall\, n \geq 2$

$\Longrightarrow h_0 = 0$ to cancel even terms

$$h(z) = h_1 z$$

Shown that $v(z) = h(z) e^{-z^2/2} \Longrightarrow v_1(z) = h_1 z e^{-z^2/2}$

Substituting $z = \sqrt{\frac{m\omega}{\hbar}}\, x \Longrightarrow u_1(x) = h_1 \sqrt{\frac{m\omega}{\hbar}}\, x\, e^{-\frac{m\omega}{2\hbar}x^2}$

Normalizing

$$\int_{-\infty}^{\infty} u_1(x)\bar{u}_1(x)\, dx = \int_{-\infty}^{\infty} h_1^2 \frac{m\omega}{\hbar} x^2 e^{-\frac{m\omega}{\hbar}x^2}$$

$$= h_1^2 \frac{m\omega}{\hbar} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2}\, dx$$

$$= h_1^2 \frac{\sqrt{\pi}}{2} \sqrt{\frac{\hbar}{m\omega}} = 1$$

$$\Longrightarrow h_1 = \left(\frac{4\, m\omega}{\pi \hbar}\right)^{1/4}$$

$$u_1(x) = \left(\frac{4\, m^3 \omega^3}{\pi \hbar^3}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

More generally, the polynomial solutions $h(z)$ to the equation

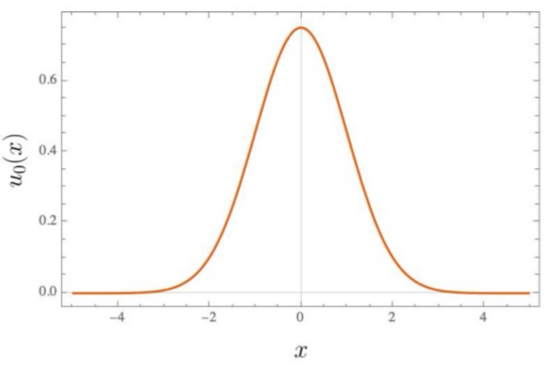
$$h''(z) - 2zh' + (\varepsilon - 1)h = 0$$

are known as Hermite polynomials usually denoted by

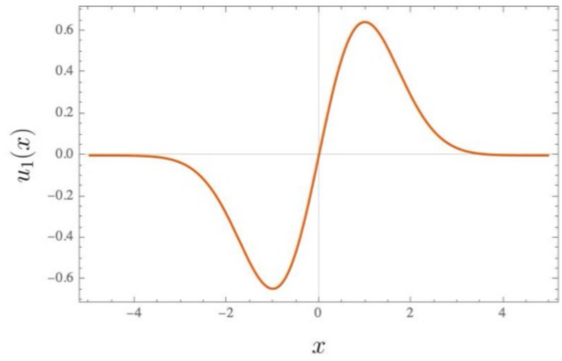
$$H_n(z)$$

Plot of wavefunctions

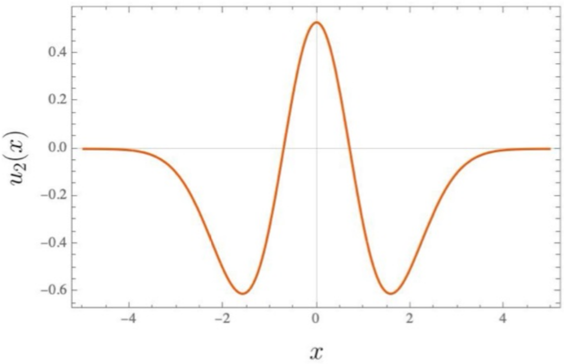
▶ $u_0(x)$:



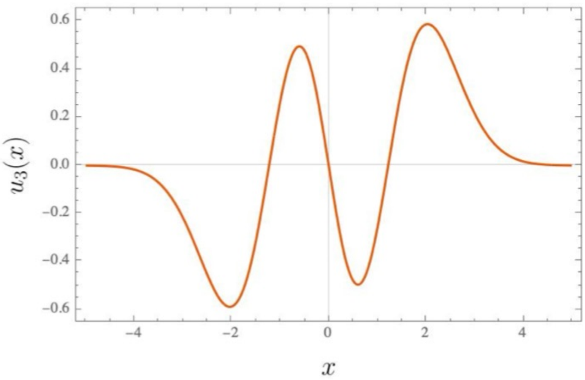
▶ $u_1(x)$:



▶ $u_2(x)$:



▶ $u_3(x)$:



THE METHOD OF FROBENIUS

Consider second-order linear ODE

$$u''(x) + p(x)u'(x) + q(x)u(x) = 0$$

If functions $p(x)$ and $q(x)$ are NOT analytic at $x = x_0$, then cannot apply Cauchy's Theorem.

However, if $x = x_0$ is a regular singularity, i.e. $(x - x_0)p(x)$ and $(x-x_0)^2 q(x)$ are analytic, then Ferdinand Georg Frobenius tells us that we can find a solution in form

$$\boxed{u(x) = \sum_{n=0}^{\infty} c_n (x - x_0)^{n+\sigma}}$$

This is established by Fuchs Theorem

Theorem Fuchs Theorem

Let x_0 be a regular singular point of the second order linear ODE

$$u''(x) + p(x)u'(x) + q(x)u(x) = 0$$

Then a solution $u(x)$ always exists and has form

$$u(x) = \sum_{n=0}^{\infty} c_n (x - x_0)^{n+\sigma} \qquad \sigma \in \mathbb{R}$$

where σ is parameter we fix

Example: Consider the equation

$$2x^2 u''(x) + x(2x+1)u'(x) - u(x) = 0 \qquad \div 2x^2$$

$$\Longrightarrow \quad u''(x) + \left(1 + \frac{1}{2}x\right)u'(x) - \frac{1}{2x^2}u(x) = 0$$

We have

$$p(x) = 1 + \frac{1}{2x}$$

$$q(x) = -\frac{1}{2x^2}$$

So $x = 0$ is a regular singular point. Hence

$$u(x) = \sum_{n=0}^{\infty} c_n (x - x_0)^{n+\sigma}$$

Differentiating

- $2x^2u''(x) = 2\sum_{n=0}^{\infty}(n+\sigma)(n+\sigma-1)c_n x^{n+\sigma}$

- $x(2x+1)u'(x) = 2\sum_{n=0}^{\infty}(n+\sigma)c_n x^{n+\sigma+1} + \sum_{n=0}^{\infty}(n+\sigma)c_n x^{n+\sigma}$
- $-u(x) = -\sum_{n=0}^{\infty} c_n x^{n+\sigma}$

Shifting summation to match powers of x,

$$2\sum_{n=0}^{\infty}(n+\sigma)c_n x^{n+\sigma+1} = 2\sum_{n=1}^{\infty}(n+\sigma-1)\, c_{n-1}\, x^{n+\sigma}$$

Now extract $n=0$ terms from other 2 so we can clump summations

$$2x^2u''(x) = 2\sigma(\sigma-1)c_0x^{\sigma} + 2\sum_{n=1}^{\infty} c_n(n+\sigma)(n+\sigma-1)x^{n+\sigma}$$

$$x(2x+1)u'(x) = \sigma c_0 x^{\sigma} + \sum_{n=1}^{\infty}\left[2(n+\sigma-1)c_{n-1} + (n+\sigma)c_n\right]x^{n+\sigma}$$

$$-u(x) = -c_0x^{\sigma} - \sum_{n=1}^{\infty} c_n x^{n+\sigma}$$

By substituting into ODE, we get

$$(2\sigma+1)(\sigma-1)x^{\sigma} + \sum_{n=1}^{\infty}\left[2(n+\sigma-1)c_{n-1} + (2n+2\sigma+1)(n+\sigma-1)\, c_n\right]x^{n+\sigma} = 0$$

All coefficients must vanish identically

$$(2\sigma+1)(\sigma-1)c_0 = 0 \qquad \text{indicial equation}$$

$$2(n+\sigma-1)c_{n-1} = -(2n+2\sigma+1)(n+\sigma-1)\, c_n$$

To avoid non-trivial solutions

$$c_0 \neq 0, \quad (2\sigma+1)(\sigma-1) = 0$$

$$\Longrightarrow \sigma = \begin{cases} -1/2 \\ 1 \end{cases}$$

The recursion relation is

$$c_n = -\frac{1}{n+\sigma+1/2}\, c_{n-1} \qquad \forall n \in \mathbb{N}$$

Simplifying by iterating

$$c_n = -\frac{1}{n+\sigma+1/2}\, c_{n-1} = \left(-\frac{1}{n+\sigma+1/2}\right)\left(-\frac{1}{n+\sigma-1/2}\right) c_{n-2}$$

$$\Longrightarrow \quad c_n = \frac{1}{\underbrace{(\sigma+3/2)(\sigma+3/2+1)\cdots\cdots(\sigma+3/2+n-1)}_{n}}\, c_0$$

The radius of convergence

$$R = \lim_{n\to\infty}\left|\frac{c_{n-1}}{c_n}\right| = \lim_{n\to\infty}\left|n+\sigma+\frac{1}{2}\right| = \infty$$

Looking at cases $\sigma = -1/2$, $\sigma = 1$,

▸ $\underline{\sigma = -1/2}$:

$$c_n = \frac{(-1)^n}{1\cdot 2\cdots\cdots n}\, c_0 = \frac{(-1)^n}{n!}\, c_0$$

and this gives us an immediate solution

$$u_1(x) = c_0\, x^{-1/2} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} x^n = c_0\, x^{-1/2} e^{-x}$$

▸ $\underline{\sigma = 1}$:

$$c_n = \frac{(-1)^n}{\underbrace{5/2\cdot 7/2\cdots \frac{2n+3}{2}}_{n}}\, c_0 = \frac{2^n(-1)^n}{1\cdot 5\cdot 7\cdots(2n+3)}\, c_0 \,\frac{\times 3}{\times 3} = \frac{3}{3}\,\frac{(-2)^n}{1\cdot 5\cdot 7\cdot 9\cdots(2n+3)}\, c_0$$

$$= \frac{3(-2)^n}{(2n+3)!!}\, c_0$$

$$\Longrightarrow \quad c_n = \frac{3(-2)^n}{(2n+3)!!}\, c_0$$

Double factorial function

$$(2k-1)!! \doteq (2k-1)(2k-3)(2k-5)\cdots 1 \qquad \forall k \in \mathbb{N}$$

Hence the second solution has form

$$u_2(x) = 3c_0 \sum_{n=0}^{\infty} \frac{(-2)^n}{(2n+3)!!} x^{n+1}$$

Using Fuch's Theorem, we found 2 linearly independent solutions.

Consider any second order linear ODE

$$u''(x) + p(x)u'(x) + q(x)u(x) = 0$$

with regular singularity at $x = x_0$

If the roots of σ_1 and σ_2 of the indicial equation, then

- $\sigma_1 - \sigma_2 \notin \mathbb{Z}$, then we have 2 linearly independent solutions
- $\sigma_1 - \sigma_2 \in \mathbb{N} \cup \{0\}$, order roots such that $\sigma_1 \geq \sigma_2$ - then there exists a power solution

$$u_1(x) = \sum_{n=0}^{\infty} c_n (x - x_0)^{n+\sigma_1}$$

together with a second solution with the following form

$$u_2(x) = \alpha u_1(x) \log(x) + \sum_{n=0}^{\infty} \tilde{c}_n (x - x_0)^{n+\sigma_2}$$

where $\alpha \in \mathbb{R}$ can be determined as a function of $\tilde{c}_0 \neq 0$ and $c_0 \neq 0$

Example: Consider the equation

$$xu''(x) + 2u'(x) + u(x) = 0$$

$$\Longrightarrow \quad u''(x) + \frac{2}{x} u'(x) + \frac{1}{x} u(x) = 0$$

- $p(x) = \frac{2}{x}$
- $q(x) = \frac{1}{x}$

Therefore $x = 0$ is a singular point

To make solving simpler, multiply through by x

$$x^2 u''(x) + 2xu'(x) + xu(x) = 0$$

Applying Fuch's Theorem

$$x^2 u''(x) = \sum_{n=0}^{\infty} (n+\sigma)(n+\sigma-1) c_n x^{n+\sigma}$$

$$2xu'(x) = 2\sum_{n=0}^{\infty} (n+\sigma) c_n x^{n+\sigma}$$

$$xu(x) = \sum_{n=0}^{\infty} c_n x^{n+\sigma+1} = \sum_{n=1}^{\infty} c_{n-1} x^{n+\sigma}$$ shifting summation

Isolating n=0 terms and combining summations

$$\sigma(\sigma+1) c_0 x^{\sigma} + \sum_{n=1}^{\infty} \left[(n+\sigma)(n+\sigma+1) c_n + c_{n-1}\right] x^{n+\sigma} = 0$$

We get indicial equation

$$\sigma(\sigma+1) = 0$$

$\Longrightarrow$ roots $\sigma_1 = 0$, $\sigma_2 = -1$

Observe $\sigma_1 - \sigma_2 = 1 \in \mathbb{N} \cup \{0\} \Longrightarrow$ apply second case, we have a logarithmic term.

▶ $\underline{\sigma_1 = 0}$: We get recursion relation

$$c_n = -\frac{1}{(n+1)(n+2)} c_n \quad \forall\, n \geq 0$$ shifting relation by 1.

$$\Longrightarrow \boxed{u_1(x) = c_0 \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,(n+1)!} x^n}$$

The radius of convergence is

$$R = \lim_{n\to\infty} \left|\frac{c_n}{c_{n+1}}\right| = \lim_{n\to\infty} (n+1)(n+2) = \infty$$

▶ $\underline{\sigma_1 = -1}$: The recursion relation ill-defined at $n=0$

$$c_{n+1} = -\frac{1}{n(n+1)} c_n$$

Setting $c_0 = 0$ and take c_1 as normalization constant reproduces $u_1(x)$, so not good.

Lets try solution of form (ansatz)

$$u_2(x) = \alpha \log(x) u_1(x) + v_2(x)$$

where

$$v_2(x) = \sum_{n=0}^{\infty} \tilde{c}_n x^{n+\sigma}$$

Differentiating

$$u_2'(x) = \alpha \frac{1}{x} u_1(x) + \alpha \log(x) u_1'(x) + v_2'(x)$$

$$u_2''(x) = -\alpha \frac{1}{x^2} u_1(x) + \alpha \frac{1}{x} u_1'(x) + \alpha \frac{1}{x} u_1'(x) + \alpha \log(x) u_1''(x) + v_2''(x)$$

Substituting into differential equation

$$\alpha \log x \underbrace{\left[x^2 u_1''(x) + 2x u_1'(x) + x u_1(x)\right]}_{0} + 2\alpha x u_1'(x) + \alpha u_1(x)$$
$$+ x^2 v_2''(x) + 2x v_2'(x) + x v_2(x) = 0$$

$$\Rightarrow x^2 v_2''(x) + 2x v_2'(x) + x v_2(x) + 2\alpha x u_1'(x) + \alpha u_1(x) = 0$$

Inserting power series for u_1 and v_2, we get

$$\sum_{n=0}^{\infty} \left[n(n+1)\tilde{c}_{n+1} + \tilde{c}_n\right] x^n + \sum_{n=0}^{\infty} \alpha(2n+1) \frac{(-1)^n}{n!(n+1)!} c_0 x^n = 0$$

Recursion relation now splits into an equation for $n=0$ and another valid for $n>0$.

$$\tilde{c}_0 = -\alpha c_0$$

$$\tilde{c}_{n+1} = -\frac{1}{n(n+1)} \tilde{c}_n - \alpha c_0 (-1)^n \frac{2n+1}{n!(n+1)!} \qquad \forall n > 0$$

Quantum Particles in 3D

The time independent Schrödinger equation in 3D is

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2 u(\vec{x}) + V(\vec{x})u(\vec{x}) = E\,u(\vec{x})}$$ TDSE in 3D

We will limit our attention to central potentials

$$V(\vec{x}) = V(r) \qquad r \doteq |\vec{x}|$$

Angular Momentum

In classical mechanics, angular momentum is

$$\vec{L} = \vec{x} \times \vec{p}$$

and for circular potentials, $\vec{L}$ is conserved, as

$$\dot{\vec{L}} = \dot{\vec{x}} \times \vec{p} + \vec{x} \times \dot{\vec{p}} \qquad \text{and} \qquad \dot{\vec{p}} = \vec{F} = -\nabla V(r)$$

$$= \cancel{\dot{\vec{x}} \times (m\dot{\vec{x}})}^{\,0} + \cancel{\vec{x} \times (-\nabla V(r))}^{\,0} \quad \text{parallel vectors}$$

and further, for circular potentials,

In classical mechanics, conservation of $\vec{L}$ is a powerful feature as from this

- direction of $\vec{L}$ is fixed $\Longrightarrow$ allows us to reduce motion from 3D to 2D since particle moves in plane determined by
$$\vec{L} \cdot \vec{x} = 0$$
- $|\vec{L}|^2$ is fixed $\Longrightarrow$ reduce problem to 1D: motion in radial direction.

SEPARATION OF VARIABLES: Quantum

Angular Momentum

In quantum, observables are operators. Hence

$$\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}}$$

and remember, action on wavefunction is

$$\hat{\vec{x}}\,u(\vec{x}) = \vec{x}\,u(\vec{x})$$

$$\hat{\vec{p}}\,u(\vec{x}) = -i\hbar\nabla u(\vec{x})$$

Computing components of the operator $\hat{L}$

$$\hat{L}_1 u(\vec{x}) = -i\hbar \left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \right) u(\vec{x})$$

$$\hat{L}_2 u(\vec{x}) = -i\hbar \left(x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \right) u(\vec{x})$$

$$\hat{L}_3 u(\vec{x}) = -i\hbar \left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right) u(\vec{x})$$

These relations can be summarized using alternating tensor

$$\varepsilon_{123} = 1 \qquad \varepsilon_{ijk} = -\varepsilon_{jik} = -\varepsilon_{kji} = -\varepsilon_{ikj}$$

$$\varepsilon_{abc} = \begin{cases} +1 & \text{if abc is an even permutation of } 1,2,3 \\ 0 & \text{if abc is not a permutation of } 1,2,3 \\ -1 & \text{if abc is an odd permutation of } 1,2,3 \end{cases}$$

The angular momentum operator can be rewritten as

$$\hat{L}_i u(\vec{x}) = -i\hbar \sum_{j,k=1}^{3} \varepsilon_{ijk} x_j \frac{\partial}{\partial x_k} u(\vec{x}) \equiv -i\hbar\, \varepsilon_{ijk} x_j \frac{\partial}{\partial x_k} u(\vec{x})$$

summation convention
repeated index

We can also define angular momentum operator as

$$\hat{L} = -\hat{p} \times \hat{x}$$

and $\hat{x} \times \hat{p} \equiv -\hat{p} \times \hat{x}$

Commutation Relations

Components of angular momentum operator do not commute amongst themselves.

Calculating the commutator

$$\boxed{[\hat{L}_i, \hat{L}_j] = \hat{L}_i \hat{L}_j - \hat{L}_j \hat{L}_i = i\hbar\, \varepsilon_{ijk} \hat{L}_k}$$

Note: The fact that $[\hat{L}_i, \hat{L}_j] \neq 0$ means particle cannot have a well-defined angular momentum in all three directions simultaneously.

If for example you know angular momentum $\hat{L}_1$, then there will be necessarily some uncertainty in the angular momentum of the other two.

The same thing happens with position and momentum

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

which tells we cannot know with infinite precision x_1, p_1 ; the uncertainty principle

The commutation relation can be proven easily. For example, for $i=1$, $j=2$

$$[\hat{L}_1, \hat{L}_2] = i\hbar\,\varepsilon_{123}\hat{L}_3 = i\hbar\hat{L}_3$$

$$[\hat{L}_1, \hat{L}_2]u(\vec{x}) = (i\hbar)^2\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right)\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right)u(\vec{x}) \;+$$

$$-(-i\hbar)^2\left(x_3\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_3}\right)\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right)u(\vec{x})$$

$$= -\hbar^2\left(x_2\frac{\partial}{\partial x_3}\,x_3\frac{\partial u(\vec{x})}{\partial x_1} - \cancel{x_1x_2\frac{\partial^2 u(\vec{x})}{\partial x_3^2}} - \cancel{x_3^2\frac{\partial^2 u(\vec{x})}{\partial x_1\partial x_2}} + x_1x_3\frac{\partial^2 u(\vec{x})}{\partial x_2\partial x_3}\right)$$

$$+\hbar^2\left(x_2x_3\frac{\partial^2 u(\vec{x})}{\partial x_1\partial x_3} - \cancel{x_3^2\frac{\partial^2 u(\vec{x})}{\partial x_1\partial x_2}} - \cancel{x_1x_2\frac{\partial^2 u(\vec{x})}{\partial x_3^2}} + x_1\frac{\partial}{\partial x_3}\frac{\partial u(\vec{x})}{\partial x_2}\right)$$

$$= -\hbar^2\left(x_2\frac{\partial u(\vec{x})}{\partial x_1} + \cancel{x_2x_3\frac{\partial^2 u(\vec{x})}{\partial x_1\partial x_2}} + \cancel{x_1x_3\frac{\partial^2 u(\vec{x})}{\partial x_2\partial x_3}}\right)$$

$$+\hbar^2\left(\cancel{x_2x_3\frac{\partial^2 u(\vec{x})}{\partial x_1\partial x_3}} + \cancel{x_1x_3\frac{\partial u(\vec{x})}{\partial x_2\partial x_3}} + x_1\frac{\partial u(\vec{x})}{\partial x_2}\right)$$

$$= i\hbar(-i\hbar)\left(x_1\frac{\partial}{\partial x_3} - x_2\frac{\partial}{\partial x_1}\right)u(\vec{x})$$

$$\equiv i\hbar\hat{L}_3\,u(\vec{x})$$

The total angular momentum operator

$$\boxed{\hat{\vec{L}}^2 = \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2}$$

This commutes with all the angular momentum components

$$\boxed{[\hat{\vec{L}}^2, \hat{L}_i] = 0 \qquad \forall i \in \{1,2,3\}}$$

This means that a quantum system can have a definite total angular momentum with a definite component of the angular momentum in some chosen reference direction, usually L_3.

We can prove this using the following identity

$$\boxed{[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}} \qquad \forall \hat{A}, \hat{B}$$

Then we get

$$[\hat{L}^2, \hat{L}_1] = [\hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2, \hat{L}_1]$$
$$= [\hat{L}_1^2, \hat{L}_1] + [\hat{L}_2^2, L_1] + [\hat{L}_3^2, \hat{L}_1]$$

Observe that

- $[\hat{L}_1^2, \hat{L}_1] = 0$ since any object commutes with itself
- $[\hat{L}_2^2, \hat{L}_1] = \hat{L}_2[\hat{L}_2, \hat{L}_1] + [\hat{L}_2, \hat{L}_1]\hat{L}_2 = -\hat{L}_2[\hat{L}_1, \hat{L}_2] - [\hat{L}_1, \hat{L}_2]\hat{L}_2 =$ $\qquad [\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

  $= i\hbar(\hat{L}_2\hat{L}_3 + \hat{L}_3\hat{L}_2)$

- $[\hat{L}_3^2, \hat{L}_1] = \hat{L}_3[\hat{L}_3, \hat{L}_1] + [\hat{L}_3, \hat{L}_1]\hat{L}_3 = i\hbar\, \varepsilon_{312}(\hat{L}_3\hat{L}_2 + \hat{L}_2\hat{L}_3) =$

  $= i\hbar(\hat{L}_3\hat{L}_2 + \hat{L}_2\hat{L}_3)$

  $= -[\hat{L}_2^2, \hat{L}_1]$

  since $\varepsilon_{312} = -\varepsilon_{132} = \varepsilon_{123} = 1$.

Hamiltonian Operator

Analyzing commutation relation between Hamiltonian operator and angular momentum operator.

The Hamiltonian operator is

central potential

$$\hat{H}u(\vec{x}) = \left(-\frac{\hbar^2}{2m}\underline{\nabla}^2 + V(r)\right)u(\vec{x})$$

This operator commutes with the angular momentum operator as potential is central

$$\boxed{[\hat{H}, \hat{L}_i] = [\hat{H}, \hat{L}^2] = 0}$$

To prove this, observe

$$[\hat{L}_i, \hat{x}_j] = i\hbar\, \varepsilon_{ijk}\hat{x}_k$$
$$[\hat{L}_i, \hat{p}_j] = i\hbar\, \varepsilon_{ijk}\hat{p}_k$$

and then using the identity $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$, we can show

$$[\hat{L}_i, \hat{\vec{x}}^2] = [\hat{L}_i, \hat{x}_1^2] + [\hat{L}_i, \hat{x}_2^2] + [\hat{L}_i, \hat{x}_3^2] = 0$$

$$[\hat{L}_i, \hat{\vec{p}}^2] = [\hat{L}_i, \hat{p}_1^2] + [\hat{L}_i, \hat{p}_2^2] + [\hat{L}_i, \hat{p}_3^2] = 0$$

These relations are all we need, since the Hamiltonian

$$\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\vec{x}^2)$$

only depends on $\hat{\vec{p}}^2$ and $\hat{\vec{x}}^2$

Theorem Common eigenfunctions of commuting operators

Two operators commute $\Longleftrightarrow$ they share the same eigenfunctions

This shows why commutations matter, especially with the Hamiltonian.

In fact, we want a solution to the 3D TDSE in terms of the Hamiltonian, reads

$$\hat{H}u(\vec{x}) = Eu(\vec{x})$$

Hence any solution is automatically an eigenfunction of the Hamiltonian. But since $\hat{H}$ commutes with both

$$\hat{\vec{L}}^2 \text{ and } \hat{L}_3$$

commutes with $\hat{H}$ and these commute amongst themselves, the solutions we are looking for can be taken to be simultaneous eigenfunctions of these 3 operators

$$\hat{H}u_{m,l,E}(\vec{x}) = E\,u_{m,l,E}(\vec{x})$$

$$\hat{\vec{L}}^2 u_{m,l,E}(\vec{x}) = l(l+1)\hbar^2 u_{m,l,E}(\vec{x})$$

$$\hat{L}_3 u_{m,l,E}(\vec{x}) = m\hbar u_{m,l,E}(\vec{x})$$

angular quantum number

The reason why we chose to parametrize the eigenvalues of $\hat{\vec{L}}^2$ as $\ell(\ell+1)$ will be clear in next section.

The Eigenfunctions

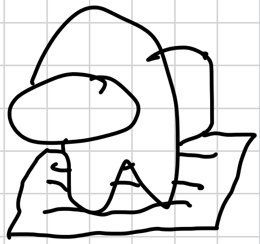
Looking at

$$\hat{H}u(\vec{x}) = \left(\frac{\hat{\vec{p}}^2}{2m} + V(|\vec{x}|)\right)u(\vec{x})$$

Since we are dealing with central potentials: use spherical co-ordinates.

Spherical polars

$$\begin{cases} x_1 = r\sin\theta\cos\phi & r \in \mathbb{R}_+ \\ x_2 = r\sin\theta\sin\phi & \theta \in [0, \pi] \\ x_3 = r\cos\theta & \phi \in [0, 2\pi] \end{cases}$$



Need to convert expressions

$$\hat{L}_1 u(\vec{x}) = -i\hbar \left(x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2} \right) u(\vec{x})$$

$$\hat{L}_2 u(\vec{x}) = -i\hbar \left(x_3 \frac{\partial}{\partial x_1} - x_1 \frac{\partial}{\partial x_3} \right) u(\vec{x})$$

$$\hat{L}_3 u(\vec{x}) = -i\hbar \left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right) u(\vec{x})$$

in terms of polar co-ordinates (r, θ, ϕ). To do so, we apply chain rule

$$\frac{\partial}{\partial x_1} f(r,\theta,\phi) = \frac{\partial r}{\partial x_1}\frac{\partial}{\partial r} f(r,\theta,\phi) + \frac{\partial \theta}{\partial x_1}\frac{\partial}{\partial \theta} f(r,\theta,\phi) + \frac{\partial \phi}{\partial x_1}\frac{\partial}{\partial \phi} f(r,\theta,\phi)$$

The partial derivatives $\partial r/\partial x_1$ and so can be found by deriving expressions with respect to x_1

(A) $1 = \sin\theta\cos\phi \dfrac{\partial r}{\partial x_1} + r\cos\theta\cos\phi \dfrac{\partial \theta}{\partial x_1} - r\sin\theta\sin\phi \dfrac{\partial \phi}{\partial x_1}$

(B) $0 = \sin\theta\sin\phi \dfrac{\partial r}{\partial x_1} + r\cos\theta\sin\phi \dfrac{\partial \theta}{\partial x_1} - r\sin\theta\cos\phi \dfrac{\partial \phi}{\partial x_1}$

(C) $0 = \cos\theta \dfrac{\partial r}{\partial x_1} - r\sin\theta \dfrac{\partial \theta}{\partial x_1}$

Taking combinations

$$[(A)\cos\phi + (B)\sin\phi]\sin\theta + (C)\cos\theta$$

$$\implies \frac{\partial r}{\partial x_1} = \sin\theta\cos\phi$$

$\dfrac{\partial r}{\partial x_2}, \dfrac{\partial r}{\partial x_3}$ similar

The end result is

$$\hat{L}_1 = i\hbar\left(\cot\theta\cos\phi\frac{\partial}{\partial\phi} + \sin\phi\frac{\partial}{\partial\theta}\right)$$

$$\hat{L}_2 = i\hbar\left(\cot\theta\sin\phi\frac{\partial}{\partial\phi} - \cos\phi\frac{\partial}{\partial\theta}\right)$$

$$\hat{L}_3 = -i\hbar\frac{\partial}{\partial\phi}$$

Total Angular momentum operator is

$$\hat{\vec{L}}^2 = \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2 = \frac{-\hbar^2}{\sin^2\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{\partial^2}{\partial\phi^2}\right]$$

Abusing notation $u(r,\theta,\phi) = u(\vec{x})$

Finding eigenfunctions

angular quantum number

$$\hat{L}_3 u(\vec{x}) = \hbar m u(\vec{x})$$

$$L_3 u(\vec{x}) = \cancel{\hbar} m u(r,\theta,\phi) = -i\cancel{\hbar}\frac{\partial}{\partial\phi}u(r,\theta,\phi)$$

$$\Longrightarrow \boxed{u(r,\theta,\phi) = Q(r,\theta)e^{im\phi}}$$

Impose $u(r,\theta,\phi+2\pi) = u(r,\theta,\phi) \Longrightarrow \boxed{m \in \mathbb{Z}}$

Now for $\hat{\vec{L}}^2$

$$\hat{\vec{L}}^2 u(r,\theta,\phi) = \cancel{\hbar^2}\ell(\ell+1)u(r,\theta,\phi)$$

$$= \frac{-\cancel{\hbar^2}}{\sin^2\theta}\left[e^{im\phi}\sin\theta\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}Q(r,\theta) + Q(r,\theta)(im)^2 e^{im\phi}\right]$$

$$\Longrightarrow -\frac{1}{\sin^2\theta}\left[e^{im\phi}\sin\theta\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}Q(r,\theta) - m^2 Q(r,\theta)\right] = \ell(\ell+1)Q(r,\theta)$$

Define $x = \cos\theta \in [-1,1]$

$$\sin\theta\frac{d}{d\theta} = \sin\theta\frac{dx}{d\theta}\frac{d}{dx} = -\sin^2\theta\frac{d}{dx} = (\cos^2\theta - 1)\frac{d}{dx} = (x^2-1)\frac{d}{dx}$$

$$\sin\theta \frac{d}{d\theta} \sin\theta \frac{d}{d\theta} = (x^2-1)\frac{d}{dx}(x^2-1)\frac{d}{dx} = (x^2-1)^2 \frac{d^2}{dx^2} + (x^2-1)2x\frac{d}{dx}$$

In terms of x and writing

$$\boxed{R(r)P(x(\theta)) = Q(r,\theta)}$$

we get

$$\frac{1}{x^2-1}\left[(x^2-1)\frac{d}{dx}(x^2-1)\frac{d}{dx} - m^2\right]P(x) = \ell(\ell+1)P(x)$$

$$\Longrightarrow \boxed{\frac{d}{dx}\left[(1-x^2)P'(x) + \ell(\ell+1)P(x) - \frac{m^2}{1-x^2}P(x) = 0\right.}$$ Associated Legendre Equation

when $m=0$

$$\boxed{\frac{d}{dx}\left[(1-x^2)P'(x)\right] + \ell(\ell+1)P(x) = 0}$$ Legendre Equation

Proposition

Let $P_\ell(x)$ be a solution to Legendre Equation with eigenvalue $\ell(\ell+1)$.

Then for any $m \in \mathbb{Z}$, the following the function

$$P_\ell^m(x) \doteq (1-x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} P_\ell(x)$$

solves the associated Legendre equation where $\frac{d}{dx}\left[(1-x^2)P_\ell'(x)\right] + \ell(\ell+1)P_\ell(x) = 0$

Legendre Equation

Differentiating Legendre equation

$$P''(x) - \frac{2x}{1-x^2}P'(x) + \frac{\ell(\ell+1)}{1-x^2}P(x) = 0 \quad \forall x \in [-1,1]$$

$$\pi(x) = \frac{-2x}{1-x^2} \qquad Q(x) = \frac{\ell(\ell+1)}{1-x^2}$$

singularities at $x_\pm = \pm 1$

Check

$$\left.\begin{aligned}&\lim_{x\to x_\pm}(x-x_\pm)\Pi(x)<\infty\\ &\lim_{x\to x_\pm}(x-x_\pm)^2 Q(x)<\infty\end{aligned}\right\}\Longrightarrow x_\pm \text{ is a regular singularity}$$

$$\boxed{\begin{aligned}&\text{Expanding around } x_\pm=\pm 1 \Longrightarrow \text{use Frobenius Method}\\ &\exists \text{ solution } P_\ell^{(\pm)}=\sum_{n=0}^{\infty} h_n (x-x_\pm)^{n+\sigma} \qquad \sigma\in\mathbb{R}\end{aligned}}$$

$x=0$ is an ordinary point $\Longrightarrow$ use Cauchy Theorem

Expanding around $x=0$

$$P(x)=\sum_{n=0}^{\infty} p_n x^n$$

Differentiating

$$P'(x)=\sum_{n=0}^{\infty} p_n n x^{n-1}$$

$$P''(x)=\sum_{n=0}^{\infty} p_n n(n-1)x^{n-2}$$

Consider

$$(1-x^2)P''(x)-2xP''(x)+\ell(\ell+1)P(x)=0$$

Substituting

$$\sum_{n=0}^{\infty} p_n n(n-1)x^{n-2}+\sum_{n=0}^{\infty}(-1)^n p_n n(n-1)x^n-2\sum_{n=0}^{\infty} p_n n x^n+\sum_{n=0}^{\infty}\ell(\ell+1)p_n x^n=0$$

Shifting index

$$\sum_{n=2}^{\infty} p_n n(n-1)x^{n-2}=\sum_{m=0}^{\infty} p_{m+2}(m+2)(m+1)x^m \qquad m=n-2\Longrightarrow n=m+2$$

$$\begin{cases} n=2 \Longrightarrow m=0\\ n=\infty \Longrightarrow m=\infty\end{cases}$$

$$=\sum_{n=0}^{\infty} p_{n+2}(n+2)(n+1)x^n$$

renaming $n\mapsto m$

Combining sums, we get

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1) p_{n+2} - (n(n+1) - l(l+1)) p_n \right] x^n = 0$$

$\Longrightarrow$ recurrence relation

$$\boxed{p_{n+2} = \frac{(n-\ell)(n+1+\ell)}{(n+2)(n+1)} p_n}$$

Radius of convergence

$$R = \lim_{n\to\infty} \left| \frac{p_n}{p_{n+1}} \right| \Longrightarrow R^2 = \lim_{n\to\infty} \left| \frac{p_n}{p_{n+1}} \right| \left| \frac{p_{n+1}}{p_{n+2}} \right| = \lim_{n\to\infty} \left| \frac{p_n}{p_{n+2}} \right|$$

$$= \left| \frac{(n+2)(n+1)}{n(n+1) - \ell(\ell+1)} \right| \longrightarrow 1 = R^2$$

$$\Longrightarrow R^2 = 1$$

$$\Longrightarrow R = 1$$

In order for power series solution to be finite at $x = \pm 1$ $\Longrightarrow$ polynomial must truncate

$\Longrightarrow$ so solution does not blow up at $x = \pm 1$

p_0 and p_1 undetermined constants

$p_0 = 0$ and $p_1 = 1$ $\Longrightarrow$ odd coefficients vanish

$$p_2 = -\frac{\ell(\ell+1)}{2}$$

For example, suppose $\ell(\ell+1) = 6$

$$p_4 = \frac{2\cdot 3 - \ell(\ell+1)}{4\cdot 3} = 0 \Longrightarrow p_6 = 0, \cdots, p_8 = 0$$

$$\Longrightarrow P_\ell(x) = 1 - 3x^2 \text{ when } \ell(\ell+1) = 6$$

In general, if $\ell(\ell+1) \in \mathbb{N}$ $\Longrightarrow$ solution is a polynomial

$$\left. \begin{array}{l} \ell = N \\ \text{or} \\ \ell = -N-1 \end{array} \right\} \Longrightarrow P_\ell(x) \text{ is a polynomial of order } x$$

$x = \cos\theta$: $\theta = 0, \pi \implies x = \pm 1$

quantization $l \in \mathbb{Z} \implies$ so polynomial truncates

solution does not blow up at $x = 1$

Solving radial equation

Given differential equation

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left[r^2R'(r)\right] + \left[-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r} + \hbar^2\frac{\ell(\ell+1)}{2m}\frac{1}{r^2}\right]R(r) = E\,R(r)$$

- $r \in [0, \infty)$
- $\lim\limits_{r\to\infty} R(r) = 0$

1) Non-Dimensionalize

$[r] = L$, $\left[\frac{d}{dr}\right] = L^{-1}$ $\quad \left[\frac{mE}{\hbar^2}\right] = L^{-2}$ $\quad \left[\frac{me^2}{\varepsilon_0\hbar^2}\right] = L^{-1}$

$[\hbar] = L\sqrt{m[E]}$

Fundamental length a

- $a^2 = -\frac{8mE}{\hbar^2}$ $\qquad [a] = \frac{1}{L}$
- $n = \frac{me^2}{2\pi\varepsilon_0\hbar^2}\frac{1}{a}$ $\qquad [n] = 1$
- $s = ar$ $\qquad [s] = 1$
- $v(s) = R(s/a)$

Substituting

$$-\frac{a^2}{s^2}\cancel{a}\frac{d}{ds}\left[\frac{s^2}{\cancel{a^2}}\cancel{a}\frac{d}{ds}v(s)\right] + \Bigg[\underbrace{-\frac{\cancel{2}m}{\hbar^2}\frac{e^2}{\cancel{4}^{\,2}\pi}\frac{a}{s}}_{=an} + \ell(\ell+1)\Bigg]v(s) = \underbrace{\frac{2mE}{\hbar^2}}_{-\frac{1}{4}a^2}v(s)$$

$$\left(\frac{1}{r} = \frac{a}{s} \qquad \frac{d}{dr} = a\frac{d}{ds}\right)$$

$\Longrightarrow$ factoring out a^2 and cancelling,

$$-\frac{1}{s^2}\frac{d}{ds}\left[s^2\frac{d}{ds}v(s)\right] + \left[-\frac{n}{s} + \frac{\ell(\ell+1)}{s^2}\right] = \frac{-1}{4}v(s)$$

2) Analyze asymptotic behavior

Look at $s \longrightarrow \infty$, we get

$$-\frac{d^2}{ds^2}v(s) - \cancelto{0}{\frac{2}{s}\frac{d}{ds}v(s)} + \left[\cancelto{0}{-\frac{n}{s} + \frac{\ell(\ell+1)}{s^2}}\right] = \frac{-1}{4}v(s)$$

In the limit $s \to \infty$

$$v''(s) - \frac{v(s)}{4} \sim 0 \quad \Longrightarrow \quad v(s) \underset{s\to\infty}{\sim} e^{\pm s/2}$$

Want want wave function to be normalizable and $\lim R(r) = 0$, so we need function to vanish

$\Longrightarrow$ choose negative exponential

$\Longrightarrow v(s) = e^{-s/2}$

Hence

$$v(s) = f(s) e^{-s/2} \quad \text{where } f \text{ is a polynomial}$$

So we have

$$-\frac{1}{s^2}\frac{d}{ds}\left[s^2 \frac{d}{ds}\left(f(s)e^{-s/2}\right)\right] + \left[-\frac{n}{s} + \ell(\ell+1)\frac{1}{s^2}\right] f(s) e^{-s/2} = -\frac{1}{4} f(s) e^{-s/2}$$

$$\Longrightarrow -\frac{1}{s^2}\frac{d}{ds}\left[s^2 e^{-s/2}\left(f'(s) - f(s)/2\right)\right] + \left[\frac{-n}{s} + \ell(\ell+1)\frac{1}{s^2}\right] f(s) e^{-s/2} = \frac{-1}{4} f(s) e^{-s/2}$$

$$\Longrightarrow -\frac{2}{s}\left(f'(s)\cancel{e^{-s/2}} - \frac{f(s)}{2}\cancel{e^{-s/2}}\right) - \left(f''(s)\cancel{e^{-s/2}} - \cancel{\frac{1}{2}f'(s)e^{-s/2}} + \cancel{\frac{1}{2}f'(s)e^{-s/2}} + \cancel{\frac{1}{4}f(s)e^{-s/2}}\right)$$
$$+ \left[\frac{-n}{s} + \ell(\ell+1)\frac{1}{s^2}\right] f(s)\cancel{e^{-s/2}} = \cancel{\frac{-1}{4} f(s) e^{-s/2}}$$

$$\Longrightarrow -\frac{2}{s} f'(s) + \frac{1}{s} f - f''(s) + f'(s) + \left[\frac{-n}{s} + \ell(\ell+1)\frac{1}{s^2}\right] f(s) = 0$$

writing in standard form

$$\boxed{f''(s) + \left(\frac{2}{s} - 1\right) f'(s) + \left(\frac{n-1}{s} - \frac{\ell(\ell+1)}{s^2}\right) f(s)}$$

$\hookrightarrow$ singularity $s=0$

3) Expand in Series

Case 1: Expand around a regular point

Case 2: Expand around a regular singular point $\longrightarrow$ Frobenius method

Consider ODE: $y''(x) + P(x)u'(x) + Q(x)u(x) = 0$

x_0 is a regular singularity $\Longrightarrow \lim\limits_{x \to x_0} (x - x_0) P(x) < \infty$

$$\lim_{x \to x_0} (x - x_0) Q(x) < \infty$$

Expanding around $s=0$, use Frobenius

$$f(s) = \sum_{m=0}^{\infty} h_m s^{m+\sigma} \qquad \sigma \in \mathbb{R}, \quad h_0 \neq 0$$

Observe

$$f'(s) = \sum_{m=0}^{\infty} h_m (m+\sigma) s^{m+\sigma-1}$$

$$f''(s) = \sum_{m=0}^{\infty} (m+\sigma)(m+\sigma-1) s^{m+\sigma-1}$$

Substituting into

$$s^2 f''(s) + (2s - s^2) f'(s) + [(n-1)s - \ell(\ell+1)] f(s) = 0$$

we get

$$\sum_{m=0}^{\infty} h_m (m+\sigma)(m+\sigma)^{-1} s^{m+\sigma} + \sum_{m=0}^{\infty} h_m 2(m+\sigma) s^{m+\sigma} + \sum_{m=0}^{\infty} (-1) h_m (m+\sigma) s^{m+\sigma+1}$$

$$+ \sum_{m=0}^{\infty} (n-1) h_m s^{m+\sigma+1} - \sum_{m=0}^{\infty} \ell(\ell+1) s^{m+\sigma}$$

2D Hydrogen atom