# Lecture 4

# Postulates of Quantum Mechanics, Operators and Mathematical Basics of Quantum Mechanics

## Reading:

## Notes and Brennan 1.3-1.6

# Postulates of Quantum Mechanics

**Classical Mechanics describes the dynamical* state variables of a particle as x, y, z, p, etc...**

**Quantum Mechanics takes a different approach. QM describes the state of any particle by an abstract "Wave Function", $\Psi( x, y ,z ,t )$, we will describe in more detail later.**

**We will introduce Five Postulates of Quantum Mechanics and one "Governing Equation", known as the Schrödinger Equation. Postulates are hypotheses that can not be proven. If no discrepancies are found in nature, then a postulate becomes an axiom or a "true statement that can not be proven". Newton's $1^{st}$ and $2^{nd}$ "Laws" and Maxwell's equations are axioms you are probably already familiar with.**

***There are also classical static variable such as mass, electronic charge, etc... that do not change during physical processes.**

# Postulates of Quantum Mechanics

## Postulate 1

**•The "Wave Function", $\Psi( x, y ,z ,t )$, fully characterizes a quantum mechanical particle including it's position, movement and temporal properties.**

**• $\Psi( x, y ,z ,t )$ replaces the dynamical variables used in classical mechanics and fully describes a quantum mechanical particle.**

**The two formalisms for the wave function:**

**•When the time dependence is included in the wavefunction, this is called the Schrödinger formulation. We will introduce a term later called an operator which is static in the Schrödinger formulation.**

**•In the Heisenberg formulation, the wavefunction is static (invariant in time) and the operator has a time dependence.**

**•Unless otherwise stated, we will use the Schrödinger formulation**

# Postulates of Quantum Mechanics

## Postulate 2

•The Probability Density Function of a quantum mechanical particle is:

$$\Psi^*( x, y ,z ,t )\Psi( x, y ,z ,t )$$

•The probability of finding a particle in the volume between v and v+dv is:

$$\Psi^*( x, y ,z ,t )\Psi( x, y ,z ,t )dv$$

•In 1D, the probability of finding a particle in the interval between x & x+dx is:

$$\Psi^*( x , t )\Psi( x, t )dx$$

•Since "$\Psi^*( x , t )\Psi( x, t )dx$" is a probability, then the sum of all probabilities must equal one. Thus,

4.1)

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = 1 \quad \text{or} \quad \int_{-\infty}^{\infty} \Psi^*(x,y,z,t)\Psi(x,y,z,t)dv = 1$$

•This is the ***<u>Normalization Condition</u>*** and is very useful in solving problems. If $\Psi$ fulfills 4.1, then $\Psi$ is said to be a normalized wavefunction.

# Postulates of Quantum Mechanics

## Postulate 2 (cont'd)

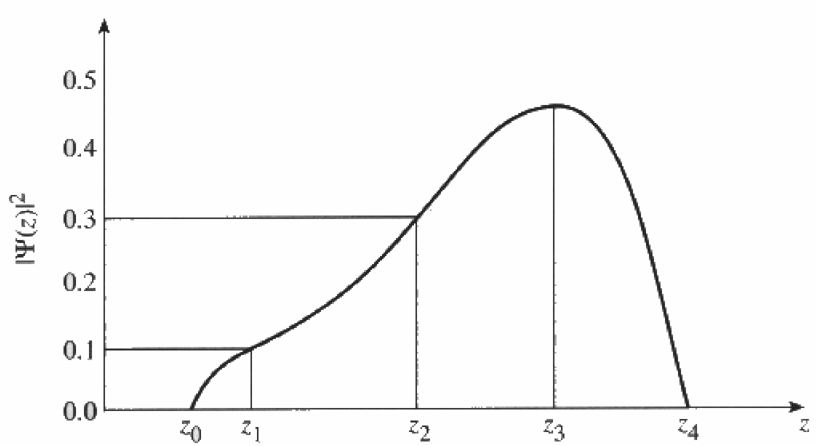
Ψ(x,y,z,t), the particle "wave function", is related to the probability of finding a particle at time t in a volume dxdydz. Specifically, this probability is:

$$\left|\Psi(x,y,z,t)\right|^2 dxdydz \text{ or } \left[\Psi^*\Psi dxdydz\right]$$

But since Ψ is a probability,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left|\Psi(x,y,z,t)\right|^2 dxdydz = 1$$

$$\text{or in 1D} \int_{-\infty}^{\infty}\left[\Psi^*\Psi dx\right] = 1$$




Introducing the concept of the wave function. $|\psi(z)|^2 dz$ proportional to the probability that the electron may be found in the interval $dz$ at the point $z$.

Solymar and Walsh figure 3.1

# Postulates of Quantum Mechanics

## Postulate 3

**Every classically obtained dynamical variable can be replaced by an "operator" that "acts on the wave function". An operator is merely the mathematical rule used to describe a certain mathematical operation. For example, the "x derivative operator" is defined as "d/dx". The wave function is said to be the operators' operand, i.e. what is being acted on.**

**The following table lists the correspondence of the classical dynamical variables and their corresponding quantum mechanical operator:**

| Classical Dynamical Variable | QM Operator Representation |
|---|---|
| Position $x$ | $x$ |
| Potential Energy $V(x)$ | $V(x)$ |
| $f(x)$ | $f(x)$ |
| Momentum $p_x$ | $\frac{\hbar}{i}\frac{\partial}{\partial x}$ |
| Kinetic Energy $\frac{p_x^2}{2m}$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ |
| $f(p_x)$ | $f\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$ |
| Total Energy (Kinetic + Potential) $E_{Total}$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$ |
| Total Energy (Time Version) $E_{Total}$ | $-\frac{\hbar}{i}\frac{\partial}{\partial t}$ |

# Postulates of Quantum Mechanics

## Postulate 4

**For each dynamical variable, ξ, there exists an expectation value, <ξ> that can be calculated from the wave function and the corresponding operator $\xi_{op}$ (see table under postulate 3) for that dynamical variable, ξ. Assuming a normalized Ψ,**

**4.2)**

$$\langle \xi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx \quad \text{or} \quad \langle \xi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,y,z,t)\xi_{op}\Psi(x,y,z,t)dv$$

**The expectation value, denoted by the braces <>, is also known as the average value or ensemble average.**

**Brennan goes through a formal derivation on pages 28-29 of the text and points out that the state of a QM particle is unknown before the measurement. The measurement forces the QM particle to be compartmentalized into a known state. However, multiple measurements can result in multiple state observances, each with a different observable. Given the probability of each state, the expectation value is a "weighted average" of all possible results weighted by each results probability.**

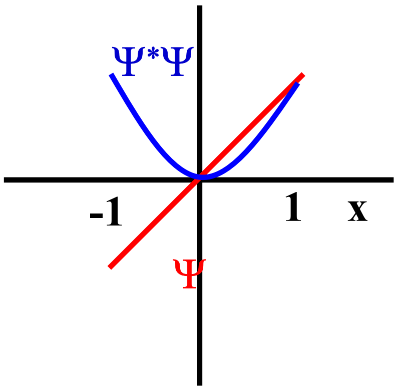
# Postulates of Quantum Mechanics

## Postulate 4

**Example: Lets assume the wave function of a QM particle is of an observable "x" is given by:**

$$\Psi(x,t)=\begin{cases} Ax & -1\le x\le 1 \\ 0 & otherwise \end{cases}$$

**We can normalize Ψ (see postulate 2) to get the constant A:**




$$1=\int_{-\infty}^{\infty}\Psi^*(x,t)\Psi(x,t)dx \quad \text{or} \quad 1=\int_{-1}^{1}A^2x^2dx$$

$$1=\frac{A^2}{3}x^3\Big|_{-1}^{1}=A^2\frac{2}{3} \quad \Rightarrow \quad A=\sqrt{\frac{3}{2}}$$

**Then we can calculate the expectation value of x, <x> as:**

$$\langle x\rangle=\int_{-1}^{1}\left[\sqrt{\frac{3}{2}}x\right]x\left[\sqrt{\frac{3}{2}}x\right]dx$$

$$\langle x\rangle=\frac{3}{2}\int_{-1}^{1}\left(x^3\right)dx=\frac{3}{2}\left(\frac{1}{4}x^4\right)\Big|_{-1}^{1}$$

$$\langle x\rangle=0$$

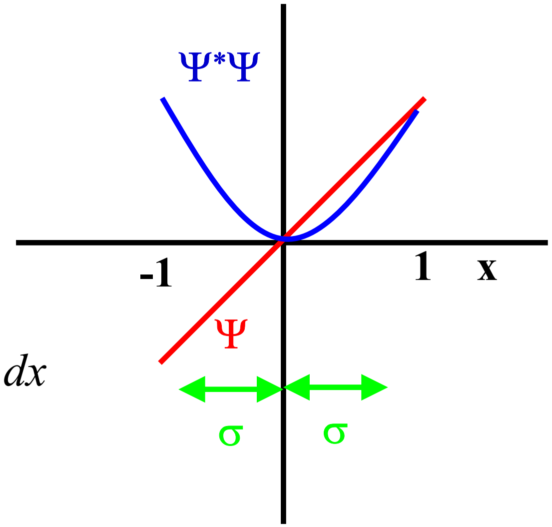
**Note: That the probability Ψ*Ψ of observing the QM particle is 0 at x=0 but multiple measurements will average to a net weighted average measurement of 0.**

# Postulates of Quantum Mechanics

## Postulate 4

**As the previous case illustrates, sometimes the "average value" of an observable is not all we need to know. Particularly, since the integrand of our <x> equation was odd, the integrand was 0. (Looking at whether a function is even or odd can often save calculation effort). We may like to also know the "standard deviation" or the variance (standard deviation squared) of the observable around the average value. In statistics, the standard deviation is:**

$$\sigma = \sqrt{\left\langle x^2 \right\rangle - \left\langle x \right\rangle^2}$$




**And since <x>=0, all we need is:**

$$\left\langle x^2 \right\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) x^2 \Psi(x,t) dx \quad \text{or} \quad \frac{3}{2}\int_{-1}^{1} x x^2 x \, dx$$

$$\left\langle x^2 \right\rangle = \frac{3}{10} x^5 \Big|_{-1}^{1} = \frac{3}{5}$$

$$\sigma = \sqrt{\left\langle x^2 \right\rangle - \left\langle x \right\rangle^2} = \sqrt{\frac{3}{5} - 0} = \sqrt{\frac{3}{5}} \approx 0.775$$

**Similarly, we could also calculate other higher order moments of distributions such as skewness, curtosis, etc...**

# Postulates of Quantum Mechanics

## Postulate 4

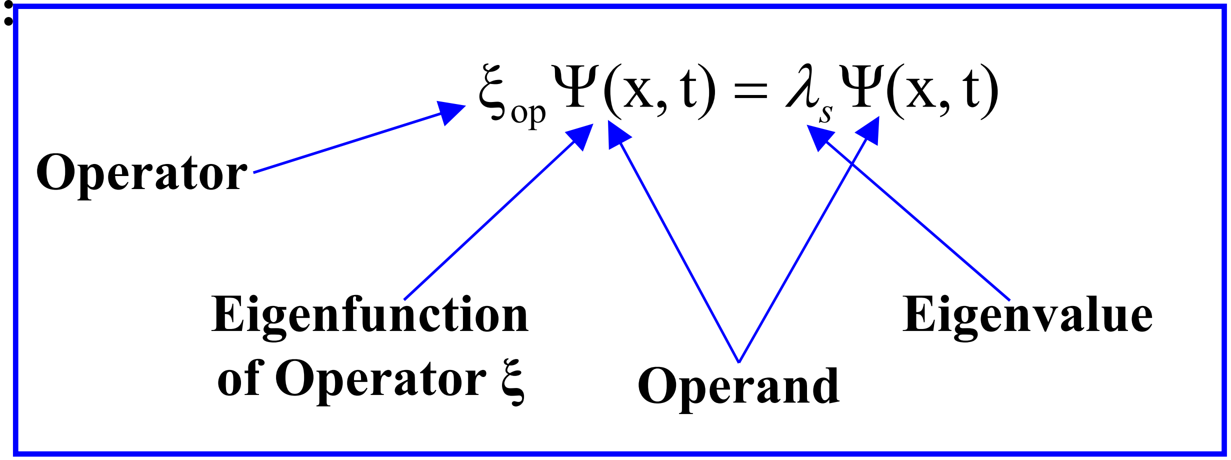
**Real world, measurable observables need to be "real" values (i.e. not imaginary / complex). What makes for a real expectation value? To answer this, we need to consider some properties of operators and develop (work toward) the concept of a "Hermitian Operator".**

**Eigenfunctions and Eigenvalues:**

**If the effect of an operator acting on an operand (wave function in our case) is such that the operand is only modified by a scalar constant, the operand is said to be an Eigenfunction of that operator and the scalar is said to be an Eigenvalue.**

**Example:**

$$\xi_{op}\Psi(x,t) = \lambda_s \Psi(x,t)$$



# Postulates of Quantum Mechanics

## Postulate 4

**Example: consider the case of an exponential function and the differential operator**

$$\xi_{op} = \frac{d}{dx}$$

$$\Psi(x,t) = e^{\lambda_s x}$$

$$\frac{d}{dx} e^{\lambda_s x} = \lambda_s e^{\lambda_s x}$$

**Eigenfunction of derivative operator**

**Operand**

**Eigenvalue**

**Eigenfunctions and Eigenvalues are very important in quantum mechanics and will be used extensively. KNOW THEM! RECOGNIZE THEM! LOVE THEM!**

# Postulates of Quantum Mechanics

## Postulate 4

## Linear Operators:

An operator is a linear operator if it satisfies the equation

$$\xi_{op} c\Psi(x,t) = c\xi_{op}\Psi(x,t)$$

where c is a constant.

$\frac{\partial}{\partial x}$ is a linear operator where as the logarithmic operator log() is not.

**Unlike the case for classical dynamical values, linear QM operators generally do not commute. Consider:**

$$\text{Classical Mechanics}: \quad xp = px$$

$$\text{Quantum Mechanics}: \quad xp_{op}\Psi(x,t) \stackrel{?}{=} p_{op}x\Psi(x,t)$$

$$x\left(\frac{\hbar}{i}\frac{d}{dx}\right)\Psi(x,t) \stackrel{?}{=} \left(\frac{\hbar}{i}\frac{d}{dx}\right)x\Psi(x,t)$$

$$x\left(\frac{\hbar}{i}\frac{d}{dx}\right)\Psi(x,t) \neq \left(\frac{\hbar}{i}\Psi(x,t)\right) + x\left(\frac{\hbar}{i}\frac{d}{dx}\right)\Psi(x,t)$$

# Postulates of Quantum Mechanics

## Postulate 4

**If two operators commute, then their physical observables can be known simultaneously.**

**However, if two operators do not commute, there exists an uncertainty relationship between them that defines the relative simultaneous knowledge of their observables. More on this later...**

# Postulates of Quantum Mechanics

**Postulate 4: A "Hermitian Operator" (operator has the property of Hermiticity) results in an expectation value that is real, and thus, meaningful for real world measurements. Another word for a "Hermitian Operator" is a "Self-Adjoint Operator". Let us work our way backwards for the 1D case:**

$$\langle \xi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx$$

If $\langle \xi \rangle$ is real and the dynamical variable is real (i.e. physically meaningful) then,

$\xi = \xi^*$ and $\langle \xi \rangle = \langle \xi^* \rangle$

This says nothing about $\xi_{op}$ as in general, $\xi_{op} \neq \xi_{op}^*$

Thus taking the conjugate of everything in the above equation,

$$\left\langle \xi^* \right\rangle = \int_{-\infty}^{\infty} \Psi(x,t)\xi_{op}^*\Psi^*(x,t)dx$$

$$\langle \xi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx = \left\langle \xi^* \right\rangle = \int_{-\infty}^{\infty} \Psi(x,t)\xi_{op}^*\Psi^*(x,t)dx$$

**This equation is simply the case where $\Psi_1=\Psi_2$**

more generally an operator is said to be hermician if it satisfies :

$$\int_{-\infty}^{\infty} \Psi_1^*(x,t)\xi_{op}\Psi_2(x,t)dx = \int_{-\infty}^{\infty} \Psi_2(x,t)\xi_{op}^*\Psi_1^*(x,t)dx$$

# Postulates of Quantum Mechanics

## Postulate 4

**Consider two important properties of a "Hermitian Operator"**

**1) Eigenvalues of Hermitian Operators are real, and thus, measurable quantities.**

**Proof:**

Hermiticity states,

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx = \int_{-\infty}^{\infty} \Psi(x,t)\xi_{op}^*\Psi^*(x,t)dx$$

Consider first the left side,

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx = \int_{-\infty}^{\infty} \Psi^*(x,t)\lambda_s\Psi(x,t)dx$$

$$= \lambda_s \int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx$$

Now consider the right hand side,

$$\int_{-\infty}^{\infty} \Psi(x,t)\xi_{op}^*\Psi^*(x,t)dx = \int_{-\infty}^{\infty} \Psi(x,t)\lambda_s^*\Psi^*(x,t)dx$$

$$= \lambda_s^* \int_{-\infty}^{\infty} \Psi(x,t)\Psi^*(x,t)dx$$

Thus, $\lambda_s = \lambda_s^*$ which is only true if $\lambda_s$ is real.

# Postulates of Quantum Mechanics

## Postulate 4

**Consider two important properties of a "Hermitian Operator"**

**2) Eigenfunctions corresponding to different and unequal Eigenvalues of a Hermitian Operator are orthogonal. Orthogonal functions of this type are important in QM because we can find a set of functions that spans the entire QM space (known as a basis set) without duplicating any information (i.e. having the one function project onto another).**

Formally, functions are orthogonal if they satisfy:

$$\int_{-\infty}^{\infty} \Psi_1^*(x,t)\Psi_2(x,t)dx = 0$$

This is true if $\xi_{op}$ is hermician and,

$$\xi_{op}\Psi_1(x,t) = \lambda_1\Psi_1(x,t) \quad \text{and} \quad \xi_{op}\Psi_2(x,t) = \lambda_2\Psi_2(x,t)$$

and $\lambda_1 \neq \lambda_2$

**See Brennan section 1.6 for details**

# Postulates of Quantum Mechanics

## Postulate 5

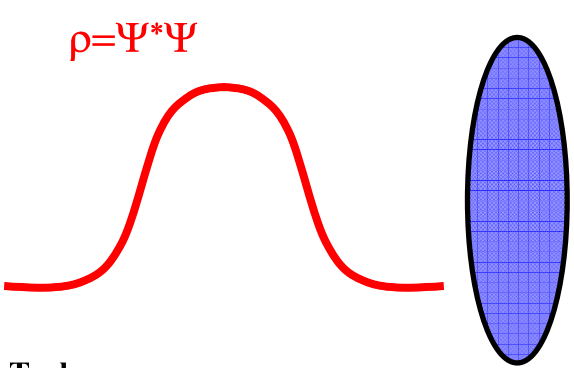
**Probability current density is conserved.**

**If a particle is not being created or destroyed it's integrated probability always remains constant (=1 for a normalized wave function). However, if the particle is moving, we can define a "Probability Current Density" and a Probability Continuity equation that describes the particles' movement through a Gaussian surface (analogous to electromagnetics). Brennan, section 1.5 derives this concept in more detail than I wish to discuss and arrives at the following:**

$$\text{Define Probability Density} \equiv \rho \equiv \Psi^*(r)\Psi(r)$$

$$\text{Define Probability Current Density (see Brennan section 1.5)} \equiv \vec{j} = \frac{\hbar}{2mi}\left(\Psi^*(r)\vec{\nabla}\Psi(r) - \Psi(r)\vec{\nabla}\Psi^*(r)\right)$$

Probability Current Density Continuity Equation




$$\vec{\nabla} \bullet \vec{j} + \frac{\partial \rho}{\partial t} = 0$$

# Postulates of Quantum Mechanics

## Postulate 5

**Basically this expression states that the wave function of a quantum mechanical particle is a smoothly varying function. In an *<u>isotropic medium</u>*, mathematically, this is stated in a simplified form as:**

$$\lim_{x \to x_o} \Psi(x,t) = \Psi(x_o,t)$$

$$and$$

$$\lim_{x \to x_o} \frac{\partial}{\partial x}\Psi(x,t) = \frac{\partial}{\partial x}\Psi(x_o,t)\Big|_{x=x_o}$$

**Simply stated, the wave function and it's derivative are smoothly varying (no discontinuities) . However, in a non-isotropic medium (examples at a heterojunction where the mass of an electron changes on either side of the junction or at an abrupt potential boundary) the full continuity equation MUST be used. Be careful as the above isotropic simplification is quoted as a Postulate in MANY QM texts but can get you into trouble (see homework problem) in non-isotropic mediums. When in doubt, use**

$$\rho \equiv \Psi^*(r)\Psi(r) \qquad \vec{j} = \frac{\hbar}{2mi}\left(\Psi^*(r)\vec{\nabla}\Psi(r) - \Psi(r)\vec{\nabla}\Psi^*(r)\right) \qquad \vec{\nabla} \bullet \vec{j} + \frac{\partial \rho}{\partial t} = 0$$

# Postulates of Quantum Mechanics

## Example using these Postulates

**Consider the existence of a wave function (Postulate 1) of the form:**

$$\Psi(x) = \begin{cases} A(1+\cos(x)) & \textit{for} \quad -\pi \le x \le \pi \\ 0 & \textit{for} \quad x \le -\pi \quad x \ge \pi \end{cases}$$

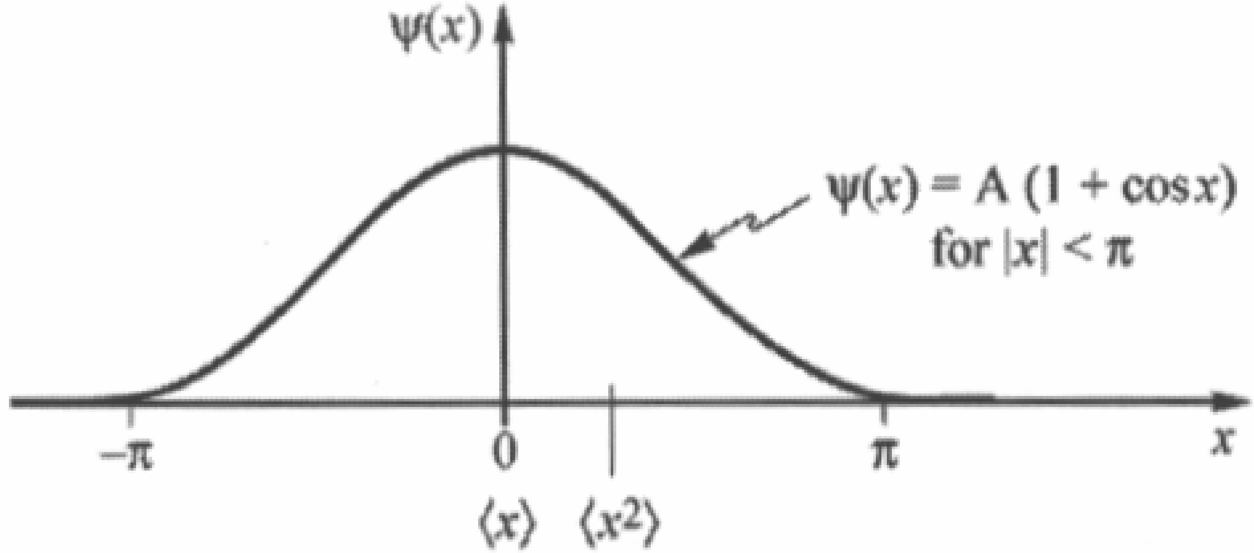



Figure after Fred Schubert with gratitude.

# Postulates of Quantum Mechanics

## Example using these Postulates

**Consider the existence of a wave function (Postulate 1) of the form:**

$$\Psi(x)=\begin{cases} A(1+\cos(x)) & \mathit{for} \quad -\pi \le x \le \pi \\ 0 & \mathit{for} \quad x \le -\pi \quad x \ge \pi \end{cases}$$

**Applying the normalization criteria from Postulate 2:**

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = 1$$

$$\int_{-\infty}^{\infty} A^2(1+\cos x)(1+\cos x)dx = 1$$

$$A^2\int_{-\pi}^{\pi}(1+2\cos x+\cos^2 x)dx = 1$$

$$A^2\left(x+2\sin x+\frac{1}{2}x+\frac{1}{4}\sin 2x\right)\Bigg|_{-\pi}^{\pi} = 1$$

$$A^2(3\pi)| = 1$$

$$A=\frac{1}{\sqrt{3\pi}}$$

$$\Psi(x)=\begin{cases} \frac{1}{\sqrt{3\pi}}(1+\cos(x)) & \mathit{for} \quad -\pi \le x \le \pi \\ 0 & \mathit{for} \quad x \le -\pi \quad x \ge \pi \end{cases}$$

# Postulates of Quantum Mechanics

## Example using these Postulates

**Show that this wave function obeys the Probability Continuity Equation (Postulate 5) at the boundaries x=+/-π:**

$$\Psi(x) = \begin{cases} \frac{1}{\sqrt{3\pi}}\left(1+\cos(x)\right) & \text{for} \quad -\pi \le x \le \pi \\ 0 & \text{for} \quad x \le -\pi \quad x \ge \pi \end{cases}$$

$$\text{Define Probability Density} \equiv \rho \equiv \Psi^*(r)\Psi(r)$$

$$\rho = \frac{1}{3\pi}\left(1 + 2\cos x + \cos^2 x\right)$$

$$\rho \text{ is independent of time so } \frac{\partial \rho}{\partial t} = 0$$

$$\text{so } \vec{\nabla}\Psi(x) = \vec{\nabla}\Psi^*(x) = -\frac{1}{\sqrt{3\pi}}\sin x$$

$$\text{Probability Current Density} \equiv \vec{j} = \frac{\hbar}{2mi}\left(\Psi^*(x)\vec{\nabla}\Psi(x) - \Psi(x)\vec{\nabla}\Psi^*(x)\right)$$

$$\vec{j} = \frac{\hbar}{2mi}\left(\left(\frac{1}{\sqrt{3\pi}}(1+\cos x)\right)\left(-\frac{1}{\sqrt{3\pi}}\sin x\right) - \left(\frac{1}{\sqrt{3\pi}}(1+\cos x)\right)\left(-\frac{1}{\sqrt{3\pi}}\sin x\right)\right) = 0$$

$$\text{Probability Current Density Continuity Equation}$$

$$\vec{\nabla} \bullet \vec{j} + \frac{\partial \rho}{\partial t} = 0 + 0 = 0$$

# Postulates of Quantum Mechanics

## Example using these Postulates

**Show that this wave function obeys the smoothness constraint (Postulate 5 for isotropic medium) at the boundaries x=+/-π:**

$$\Psi(x) = \begin{cases} \frac{1}{\sqrt{3\pi}}(1+\cos(x)) & for \quad -\pi \le x \le \pi \\ 0 & for \quad x \le -\pi \quad x \ge \pi \end{cases}$$

$$\left[\begin{array}{c} Lim \\ x \to \pi \ \ (\text{or} - \pi) \end{array}\right] \frac{1}{\sqrt{3\pi}}(1+\cos x) = \frac{1}{\sqrt{3\pi}}(1+\cos\pi)$$

$$0 = 0 \text{ for x} = -\pi \text{ or } \pi$$

$$and$$

$$\left[\begin{array}{c} Lim \\ x \to \pi \ \ (\text{or} - \pi) \end{array}\right] -\frac{1}{\sqrt{3\pi}}\sin x = -\frac{1}{\sqrt{3\pi}}\sin\pi$$

$$0 = 0 \text{ for x} = -\pi \text{ or } \pi$$

**Thus, the wave function and its derivative are both zero and continuous at the boundary (same for x=-π).**

# Postulates of Quantum Mechanics

## Example using these Postulates

**What is the expected position of the particle? (Postulate 3)**

$$\Psi(\mathrm{x}) = \begin{cases} \frac{1}{\sqrt{3\pi}}(1+\cos(\mathrm{x})) & \mathit{for} \quad -\pi \le \mathrm{x} \le \pi \\ 0 & \mathit{for} \quad \mathrm{x} \le -\pi \quad \mathrm{x} \ge \pi \end{cases}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi dx$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \frac{1}{\sqrt{3\pi}}(1+\cos x) x \frac{1}{\sqrt{3\pi}}(1+\cos x) dx$$

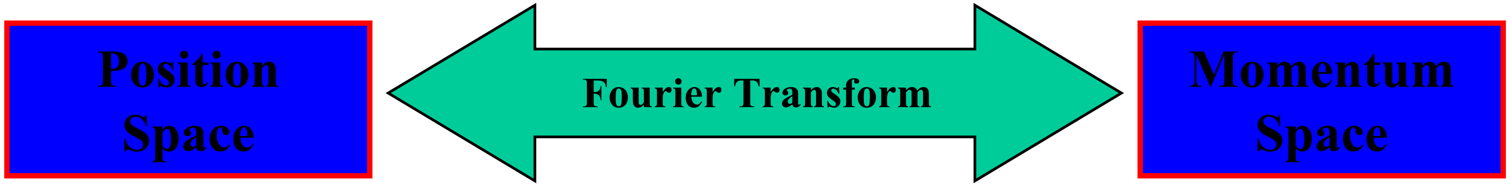
$$\langle x \rangle = \frac{1}{3\pi} \int_{-\pi}^{\pi} (1 + 2\cos x + \cos^2 x) x dx$$

**Since the function in parenthesis is even and "x" is odd, the product (integrand) is odd between symmetric limits of x=+/-π). Thus,**

$$\langle x \rangle = 0$$

**Note: Postulate 4 is not demonstrated because Ψ is not an Eigenfunction of any operator.**

# Momentum-Position Space and Transformations




$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{ipx/\hbar} dp \qquad \Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) e^{-ipx/\hbar} dx$$

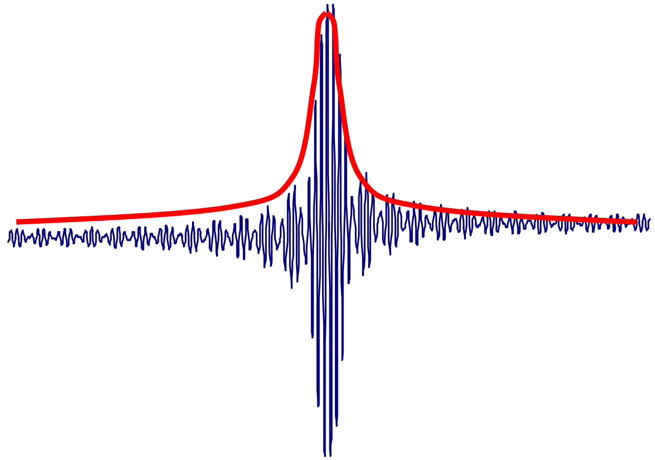
If $\Psi(\mathrm{x})$ is normalized then so is $\Phi(\mathrm{p})$

$$\int_{-\infty}^{\infty} \Psi^*(\mathrm{x})\Psi(\mathrm{x})d\mathrm{x} = \int_{-\infty}^{\infty} \Phi^*(\mathrm{p})\Phi(\mathrm{p})d\mathrm{p} = 1$$

If a state is localized in position, x, it is delocalized in momentum, p. This leads us to a fundamental quantum mechanical principle: You can not have infinite precision measurement of position and momentum simultaneously. If the momentum (and thus wavelength from $p=h/\lambda$) is known, the position of the particle is unknown and vice versa.

For more detail, see Brennan p. 24-27

# Momentum-Position Space and Transformations

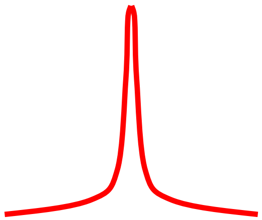


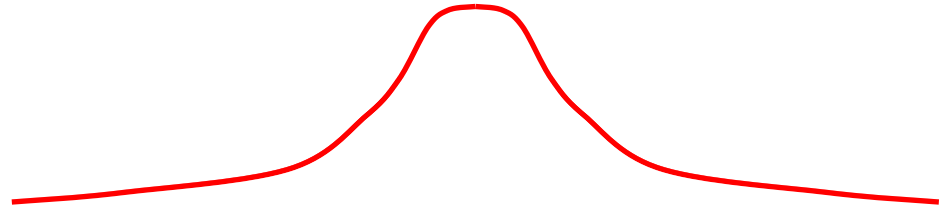
$$\Psi(x) = e^{\frac{-x^2}{2b^2}} \quad \longleftrightarrow \quad \phi(p) = be^{\frac{-b^2 p^2}{2\hbar^2}}$$

**Fourier Transform**

The above wave function is a superposition of 27 simple plane waves and creates a net wave function that is localized in space. The red line is the amplitude envelope (related to $\Psi^*\Psi$). These types of wave functions are useful in describing particles such as electrons. The wave function envelope can be approximated with a Gaussian function in space. Using the Fourier relationship between space and momentum, this can be transformed into a Gaussian in momentum (see Brennan section 1.3). The widths of the two Gaussians are inversely related.

# Momentum-Position Space and Transformations





$$\Psi(x) = e^{\frac{-x^2}{2b^2}}$$

**Fourier Transform**

$$\phi(p) = b e^{\frac{-b^2 p^2}{2\hbar^2}}$$

The widths of the two Gaussians are inversely related. Thus, accurate knowledge of position leads to inaccurate knowledge of momentum.

# Uncertainty And the Heisenberg Uncertainty Principle

**Due to the probabilistic nature of Quantum Mechanics, uncertainty in measurements is an inherent property of quantum mechanical systems. Heisenberg described this in 1927.**

**For any two Hermitian operators that do not commute (i.e. $B_{OP}A_{OP} \neq A_{OP}B_{OP}$ ) there observables A and B can not be simultaneously known (see Brennan section 1.6 for proof). Thus, there exists an uncertainty relationship between observables whose Hermitian operators do not commute.**

**Note: if operators A and B do commute (i.e. AB=BA) then the observables associated with operators A and B can be known simultaneously.**

# Uncertainty And the Heisenberg Uncertainty Principle

**Consider the QM variable, $\xi$, with uncertainty (standard deviation) $\Delta\xi$ defined by the variance (square of the standard deviation or the mean deviation),**

$$(\Delta\xi)^2 = <\xi^2> - <\xi>^2$$

**$\Delta\xi$ is the standard/mean deviation for the variable $\xi$ from its expectation value $<\xi>$**

**There are two derivations of the Heisenberg Uncertainty Principle in QM texts. The one in Brennan is more precise, but consider the following derivation for it's insight into the nature of the uncertainty. Brennan's derivation will follow.**

# Uncertainty And the Heisenberg Uncertainty Principle

**Insightful Derivation:**

**Consider a wave function with a Gaussian distribution defined by:**

$$\Psi(x) = \frac{A_x}{(\Delta\xi)\sqrt{2\pi}} e^{\frac{-x^2}{2(\Delta\xi)^2}}$$

**The normalization constant can be determined as,**

$$A_x = (4\pi)^{1/4}\sqrt{(\Delta\xi)}$$

**Taking the Fourier transformation of this function into the momentum space we get,**

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) e^{-ipx/\hbar} dx$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \left( \frac{(4\pi)^{1/4}\sqrt{(\Delta\xi)}}{(\Delta\xi)\sqrt{2\pi}} e^{\frac{-x^2}{2(\Delta\xi)^2}} \right) e^{-ipx/\hbar} dx$$

$$\Phi(p) = (4\pi)^{1/4}\sqrt{\frac{\hbar}{(\Delta\xi)}} \frac{1}{\sqrt{2\pi}\left(\frac{\hbar}{(\Delta\xi)}\right)} e^{\frac{-p^2}{2\left(\hbar/(\Delta\xi)\right)^2}}$$

The standard deviation in momentum space is inversely related to the standard deviation in position space.

# Uncertainty And the Heisenberg Uncertainty Principle

**Insightful Derivation:**

**The standard deviation in momentum space is inversely related to the standard deviation in position space.**

**Defining:** $\sigma_x = (\Delta\xi)$ and $\sigma_\mathrm{p} = \hbar/(\Delta\xi)$

**Position Space**

$$\Psi(x) = \frac{(4\pi)^{1/4}\sqrt{\sigma_X}}{\sigma_X\sqrt{2\pi}}\, e^{\frac{-x^2}{2(\sigma_X)^2}}$$

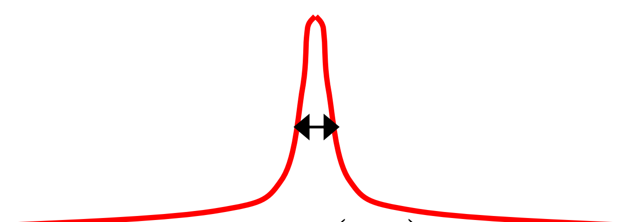
$$\Psi(x) = \frac{(4\pi)^{1/4}}{\sqrt{\sigma_X}\sqrt{2\pi}}\, e^{\frac{-x^2}{2(\sigma_X)^2}}$$

**Momentum Space**

$$\Phi(p) = \frac{(4\pi)^{1/4}\sqrt{\sigma_p}}{\sigma_p\sqrt{2\pi}}\, e^{\frac{-p^2}{2(\sigma_p)^2}}$$

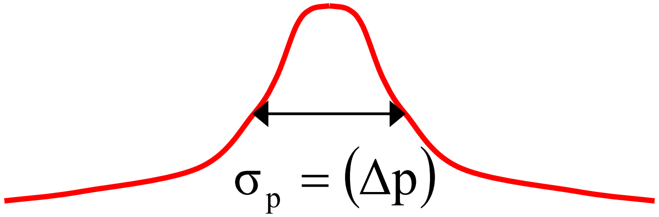
$$\Phi(p) = \frac{(4\pi)^{1/4}}{\sqrt{\sigma_p}\sqrt{2\pi}}\, e^{\frac{-p^2}{2(\sigma_p)^2}}$$

$$\sigma_\mathrm{x} = (\Delta\mathrm{x}) \text{ and } \sigma_\mathrm{p} = (\Delta\mathrm{p})$$



$\sigma_\mathrm{x} = (\Delta\mathrm{x})$

$$\boxed{\Delta\mathrm{x}\Delta\mathrm{p} = \hbar}$$



$\sigma_\mathrm{p} = (\Delta\mathrm{p})$

# Uncertainty And the Heisenberg Uncertainty Principle

**Precise Derivation:**

**The solution for the Gaussian distribution is exact only for that distribution. However, the assumption of a Gaussian distribution overestimates the uncertainty in general. Brennan (p. 46-48) derives the precise "General" Heisenberg Uncertainty Relationship using:**

**A) If two operators do not commute (i.e. AB≠BA) in general a relationship can be written such that AB-BA=iC**

**B) Given (A) the following property proven true by Merzbacher 1970:**

$$(\Delta A)^2 (\Delta B)^2 \geq 0.25C^2$$

**Thus, given the position operator, x, and momentum operator, $p_x=(\hbar/i)(d/dx)$,**

$$xp_x - p_x x = iC$$

Letting this operate on wave function Ψ

$$\left(xp_x - p_x x\right)\Psi = iC\Psi$$

$$\left(x\frac{\hbar}{i}\frac{d}{dx} - \frac{\hbar}{i}\frac{d}{dx}x\right)\Psi = iC\Psi$$

# Uncertainty And the Heisenberg Uncertainty Principle

**Precise Derivation (cont'd):**

**A) If two operators do not commute (i.e. AB≠BA) in general a relationship can be written such that AB-BA=iC**

**B) Given (A) the following property proven true by Merzbacher 1970:**

$$(\Delta A)^2 (\Delta B)^2 \geq 0.25C^2$$

$$xp_x - p_x x = iC$$

Letting this operate on wave function Ψ

$$\left(xp_x - p_x x\right)\Psi = iC\Psi$$

$$\left(x\frac{\hbar}{i}\frac{d}{dx} - \frac{\hbar}{i}\frac{d}{dx}x\right)\Psi = iC\Psi$$

$$x\frac{\hbar}{i}\frac{d}{dx}\Psi - \frac{\hbar}{i}\frac{d}{dx}\left(x\Psi\right) = iC\Psi$$

$$\left(x\frac{\hbar}{i}\frac{d}{dx}\Psi\right) - \frac{\hbar}{i}\Psi - \left(x\frac{\hbar}{i}\frac{d}{dx}\Psi\right) = iC\Psi$$

$$-\frac{\hbar}{i}\Psi = iC\Psi$$

$$\hbar = C$$

# Uncertainty And the Heisenberg Uncertainty Principle

**Precise Derivation (cont'd)**

**Thus, since $(\Delta A)^2 (\Delta B)^2 \geq 0.25C^2$, with in this case, $\Delta A=\Delta x$ and $\Delta B=\Delta p$,**

$$xp_x - p_x x = i\hbar$$

For this case, the uncertainies associated with x is $\Delta x$, and $p_x$ is $\Delta p$ must be related to $\hbar$

$$(\Delta x)^2 (\Delta p)^2 \geq \left(\frac{\hbar}{2}\right)^2$$

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$$

Note the extra factor of ½.

# Uncertainty And the Heisenberg Uncertainty Principle

## Energy Time Derivation:

**Using: Group Velocity, $v_{group}=\Delta x/\Delta t=\Delta\omega/\Delta k$ and the de Broglie relation $\Delta p=\hbar\Delta k$ and the Planck Relationship $\Delta E=\hbar\Delta\omega$:**

$$(\Delta x)(\Delta p) \geq \frac{\hbar}{2}$$

**Using Group Velocity** →
$$\left(\frac{\Delta t \Delta \varpi}{\Delta k}\right)(\Delta p) \geq \frac{\hbar}{2}$$

**Using de Broglie relation** →
$$\left(\frac{\Delta t \Delta \varpi}{\Delta k}\right)(\hbar \Delta k) \geq \frac{\hbar}{2}$$

$$(\Delta t)(\Delta \varpi) \geq \frac{1}{2}$$

**Using Planck Relationship** →
$$(\Delta t)\left(\frac{\Delta E}{\hbar}\right) \geq \frac{1}{2}$$

$$\boxed{(\Delta t)(\Delta E) \geq \frac{\hbar}{2}}$$

# Operators in Momentum Space

## Postulate 3 (additional information)

**Equivalent "momentum space operators" for each real space counterpart.**

| Classical Dynamical Variable | QM Operator Real Space Representation | QM Operator Momentum Space Representation |
| --- | --- | --- |
| Position $x$ | $x$ | $-\frac{\hbar}{i}\frac{\partial}{\partial p_x}$ |
| Potential Energy $V(x)$ | $V(x)$ | $V\left(-\frac{\hbar}{i}\frac{\partial}{\partial p_x}\right)$ |
| $f(x)$ | $f(x)$ | $f\left(-\frac{\hbar}{i}\frac{\partial}{\partial p_x}\right)$ |
| Momentum $p_x$ | $\frac{\hbar}{i}\frac{\partial}{\partial x}$ | $p_x$ |
| Kinetic Energy $\frac{p_x^2}{2m}$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ | $\frac{p_x^2}{2m}$ |
| $f(p_x)$ | $f\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$ | $f(p_x)$ |
| Total Energy (Kinetic + Potential) $E_{Total}$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)$ | $\frac{p_x^2}{2m}+V\left(-\frac{\hbar}{i}\frac{\partial}{\partial p_x}\right)$ |
| Total Energy (Time Version) $E_{Total}$ | $-\frac{\hbar}{i}\frac{\partial}{\partial t}$ | $-\frac{\hbar}{i}\frac{\partial}{\partial t}$ |

# Dirac Notation

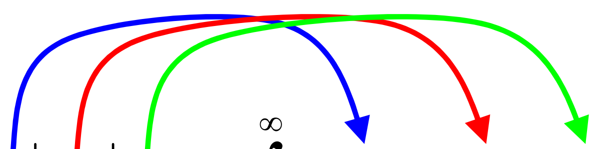
**There exists a short hand notation known as Dirac notation that simplifies writing of QM equations and is valid in either position or momentum space.**

$$\langle \Psi | \xi_{op} | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx$$

or in momentum space,

$$\langle \Psi | \xi_{op} | \Psi \rangle = \int_{-\infty}^{\infty} \Phi^*(p,t)\xi_{op}\Phi(p,t)dp$$

**Note: The left side, <Ψ, is known as a "Bra" while the right side, Ψ>, is known as a "ket" (derived from the "Bracket" notation). The "ket" is by definition, the complex conjugate of the argument.**



$$\langle \Psi | \xi_{op} | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx$$

**Dirac notation is valid in either position or momentum space so the variables, x, y, z, t, and p can be optionally left out.**

# Dirac Notation

**The operator acts on the function on the right side:**

$$\langle \Psi | \xi_{op} | \Psi \rangle = \langle \Psi | \xi_{op} \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\xi_{op}\Psi(x,t)dx$$

**If you need the operator to act on the function to the left, write it explicitly.**

$$\langle \xi_{op}\Psi_1 | \Psi_2 \rangle = \int_{-\infty}^{\infty} \Psi_2(x,t)\xi^*_{op}\Psi^*_1(x,t)dx$$

**Note that in this example, we have commuted the left hand side (operator and $\Psi_1$) with the right hand side ($\Psi_2$). This is okay. While not all operators commute, any function times another function does commute (i.e. once the operator conjugate has acted on the $\Psi_1$* , the result is merely a function which always commutes). Thus, it is the operator that may or may not commute but the functions that result from an operator acting on a wave function always commute.**

# Dirac Notation

**The Dirac form of Hermiticity is:**

$$\int_{-\infty}^{\infty} \Psi_1^{*}(x,t)\xi_{op}\Psi_2(x,t)dx = \int_{-\infty}^{\infty} \Psi_2(x,t)\xi^{*}{}_{op}\Psi_1^{*}(x,t)dx$$

$$\langle \Psi_1 | \xi_{op} | \Psi_2 \rangle = \langle \Psi_2 | \xi_{op} | \Psi_1 \rangle^{*}$$

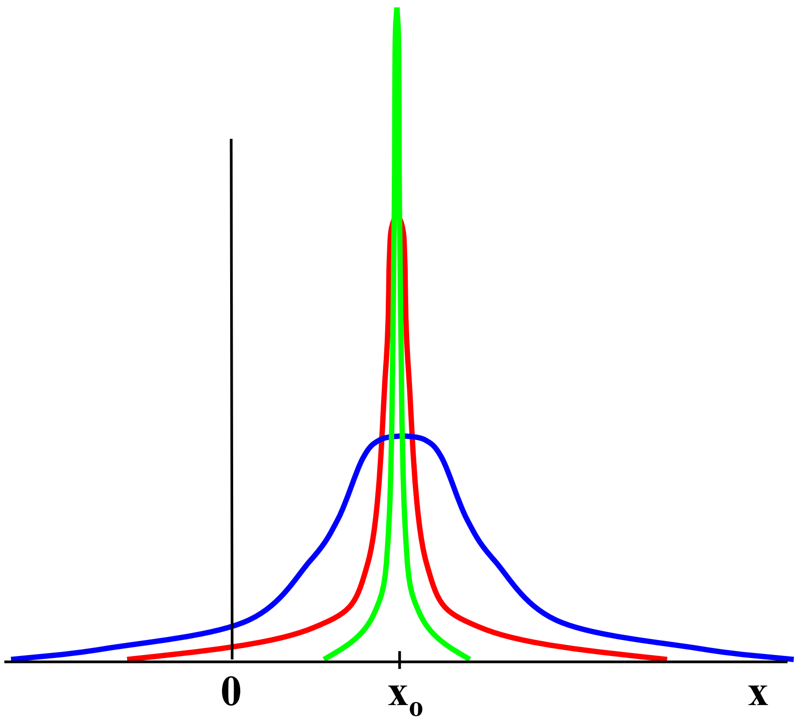
*or*

$$\left\langle \Psi_1 \middle| \xi_{op}\Psi_2 \right\rangle = \langle \xi_{op}\Psi_1 | \Psi_2 \rangle$$

# Dirac Delta Function

**The Dirac Delta Function is:**

$$\delta(x-x_o) \equiv \lim_{\sigma\to 0} \frac{1}{\sigma\sqrt{2\pi}} e^{\left(-\frac{1}{2}\left(\frac{x-x_o}{\sigma}\right)^2\right)}$$




$$\delta(x-x_o) = \infty \qquad \text{for } x = x_o$$

$$\delta(x-x_o) = 0 \qquad \text{for } x \neq x_o$$

$$\int_{-\infty}^{\infty} \delta(x-x_o)dx = 1$$

**Some useful properties of the delta function are:**

$$\delta(x) = \delta(-x)$$

$$\delta(ax) = \frac{1}{a}\delta(x)$$

$$f(x)\delta(x-x_o) = f(x_o)\delta(x-x_o)$$

$$\delta(x-x_o) = 0 \qquad \text{for } x \neq x_o$$

$$\int_{-\infty}^{\infty} f(x)\delta(x-x_o)dx = f(x_o)$$

$$\int_{-\infty}^{\infty} f(x)\frac{d}{dx}\delta(x-x_o)dx = -\frac{d}{dx}f(x)\Big|_{x=x_o}$$

# Dirac and Kronecker Delta Function

**The Dirac Delta Function is:**

$$\delta(x - x_o) \equiv \begin{cases} 1 \text{ for } x = x_o \\ 0 \text{ otherwise} \end{cases}$$

**The Kronecker Delta Function is:**

$$\delta_{ij} \equiv \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$