PHYS 304

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Preliminaries

Spherical coordinates

$$\begin{cases} x = r\sin(\theta)\cos(\phi) \\ y = r\sin(\theta)\sin(\phi) \\ z = r\cos(\theta) \end{cases} \qquad \begin{cases} r = \sqrt{x^2+y^2+z^2} \\ \theta = \arctan\left(\sqrt{x^2+y^2}/z\right) \\ \phi = \arctan(y/x) \end{cases}$$

θ is the polar angle, measured from $+z$ axis. ϕ is the azimuthal angle, measured from the $+x$ axis. Cartesian basis $\underline{e}_i$ are dependent on $\underline{s}_j(r,\theta,\phi)$

$$\begin{cases} \underline{e}_1 = \sin(\theta)\cos(\phi)\underline{s}_1 + \cos(\theta)\cos(\phi)\underline{s}_2 - \sin(\phi)\underline{s}_3 \\ \underline{e}_2 = \sin(\theta)\sin(\phi)\underline{s}_1 + \cos(\theta)\sin(\phi)\underline{s}_2 + \cos(\phi)\underline{s}_3 \\ \underline{e}_3 = \cos(\theta)\underline{s}_1 - \sin(\theta)\underline{s}_2 \end{cases}$$

Spherical basis in terms of Cartesian basis

$$\begin{cases} \underline{s}_1 = \sin(\theta)\cos(\phi)\underline{e}_1 + \sin(\theta)\sin(\phi)\underline{e}_2 + \cos(\theta)\underline{e}_3 \\ \underline{s}_2 = \cos(\theta)\cos(\phi)\underline{e}_1 + \cos(\theta)\sin(\phi)\underline{e}_2 - \sin(\theta)\underline{e}_3 \\ \underline{s}_3 = -\sin(\phi)\underline{e}_1 + \cos(\phi)\underline{e}_2 \end{cases}$$

$\underline{s}_i$ are dependent on r,θ,ϕ themselves.

$$dV = dx\,dy\,dz \mapsto r^2\sin(\theta)\,dr\,d\theta\,d\phi$$

Gradient

$$\underline{\nabla} u = \frac{\partial u}{\partial r}\underline{s}_1 + \frac{1}{r}\frac{\partial u}{\partial \theta}\underline{s}_2 + \frac{1}{r\sin(\theta)}\frac{\partial u}{\partial \phi}\underline{s}_3$$

Divergence

$$\underline{\nabla}\cdot\underline{u} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 u_r\right) + \frac{1}{r\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)u_\theta\right) + \frac{1}{r\sin(\theta)}\frac{\partial u_\phi}{\partial\theta}$$

Curl

$$\underline{\nabla}\times\underline{u} = \frac{1}{r\sin(\theta)}\left[\frac{\partial}{\partial\theta}\left(\sin(\theta)u_\phi\right) - \frac{\partial u_\theta}{\partial\phi}\right]\underline{s}_1 + \frac{1}{r}\left[\frac{1}{\sin(\theta)}\frac{\partial u_r}{\partial\phi} - \frac{\partial}{\partial r}\left(ru_\phi\right)\right]\underline{s}_2 + \frac{1}{r}\left[\frac{\partial}{\partial r}\left(ru_\theta\right) - \frac{\partial u_r}{\partial\theta}\right]\underline{s}_3$$

Laplacian

$$\nabla^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial u}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2 u}{\partial\phi^2}$$

Cylindrical coordinates

$$\begin{cases} x = r\cos(\phi) \\ y = r\sin(\phi) \\ z = z \end{cases} \qquad \begin{cases} r = \sqrt{x^2+y^2} \\ \phi = \arctan(y/x) \\ z = z \end{cases}$$

r is the distance to the closest point on the z axis (different from spherical coordinates). ϕ is the azimuthal angle, measured from the $+x$ axis.

$$\begin{cases} \underline{e}_1 = \cos(\phi)\underline{s}_1 - \sin(\phi)\underline{s}_2 \\ \underline{e}_2 = \sin(\phi)\underline{s}_1 + \cos(\phi)\underline{s}_2 \\ \underline{e}_3 = \underline{s}_3 \end{cases} \qquad \begin{cases} \underline{s}_1 = \cos(\phi)\underline{e}_1 + \sin(\phi)\underline{e}_2 \\ \underline{s}_2 = -\sin(\phi)\underline{e}_1 + \cos(\phi)\underline{e}_2 \\ \underline{s}_3 = \underline{e}_3 \end{cases}$$

$$dx\,dy\,dz \mapsto r\,dr\,d\phi\,dz$$

Gradient

$$\underline{\nabla} u = \frac{\partial u}{\partial r}\underline{s}_1 + \frac{1}{r}\frac{\partial u}{\partial\phi} + \frac{\partial u}{\partial z}\underline{s}_3$$

Divergence

$$\underline{\nabla}\cdot\underline{u} = \frac{1}{r}\frac{\partial}{\partial r}(ru_1) + \frac{1}{r}\frac{\partial u_2}{\partial\phi} + \frac{\partial u_3}{\partial z}$$

Curl

$$\underline{\nabla}\times\underline{u} = \left[\frac{1}{r}\frac{\partial u_3}{\partial\phi} - \frac{\partial u_2}{\partial z}\right]\underline{s}_1 + \left[\frac{\partial u_1}{\partial z} - \frac{\partial u_3}{\partial r}\right]\underline{s}_2 + \frac{1}{r}\left[\frac{\partial}{\partial r}(ru_2) - \frac{\partial u_1}{\partial\phi}\right]\underline{s}_3$$

Laplacian

$$\nabla^2 u = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial\phi^2} + \frac{\partial^2 u}{\partial z^2}$$

Vectors

A vector space is a set of vectors, $(|\alpha\rangle, |\beta\rangle, \dots)$ a set of scalars, $(a, b, \cdots)$, that is closed under vector addition and scalar multiplication.

- α, β are labels for some vector. We can equally label vectors by numbers, such as $|1\rangle$

The set $|\alpha\rangle, |\beta\rangle, \dots$ is *linearly independent* if the only combination that gives the zero vector

$$a|\alpha\rangle + b|\beta\rangle + \cdots = \underline{0}$$

is for all $a, b, \cdots = 0$.

Given a n dimension basis,

$$|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle$$

we can always expand vectors in a linear combination of the basis vectors:

$$|\alpha\rangle = \sum_{i=1}^{n} a_i |e_i\rangle$$

The coefficients a_i for $n = 1, 2, \dots, n$ are the components of $|\alpha\rangle$ under a particular basis.

Inner Products

A vector space endowed with an inner product is also an *inner product space*.We denote the inner product of $|\alpha\rangle$ and $|\beta\rangle$ as $\langle\alpha|\beta\rangle$.

- Noncommutative: $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$
- Distributive: $\langle\alpha|(b|\beta\rangle + c|\gamma\rangle)\rangle = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle$
- $\langle\alpha|\alpha\rangle \geq 0$
- $\langle\alpha|\alpha\rangle = 0$ iff $|\alpha\rangle = 0$
- $\|\alpha\|^2 = \langle\alpha|\alpha\rangle$

A set of vectors is orthonormal when

$$\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$$

Its always possible to choose an orthonormal basis to express our vectors in. With an orthonormal basis,

$$\langle\alpha|\beta\rangle = \sum_{i=1}^{n} a_i^* \beta_i$$

Under the inner product:

- Multiplication by a constant:

$$\langle c\alpha|\beta\rangle = c^*\langle\alpha|\beta\rangle$$
$$\langle\alpha|c\beta\rangle = c\langle\alpha|\beta\rangle$$

- For a linear transformation $\hat{T}$:

$$\langle\hat{T}\alpha|\beta\rangle = \left\langle\alpha\middle|\hat{T}^\dagger\beta\right\rangle$$
$$\left\langle\hat{T}^\dagger\alpha\middle|\beta\right\rangle = \langle\alpha|\hat{T}\beta\rangle$$

We are abusing the notation here: $\langle\hat{T}\alpha|\beta\rangle$. Since α, β are labels, not vectors. $\hat{T}$ acting on a label has no meaning. $\hat{T}\beta$ means $\hat{T}|\beta\rangle$.The following are unproven:

Schwarz inequality:

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle$$

Matrices

All operators in quantum mechanics are linear transformations.

A transformation is linear when

$$\hat{T}\left(a\left|\alpha\right\rangle + b\left|\beta\right\rangle\right) = a\hat{T}\left|\alpha\right\rangle + b\hat{T}\left|\beta\right\rangle$$

If we know how $\hat{T}$ transforms a basis, we can find out how it will transform any vectors expressible by that basis

$$\hat{T}\left|e_j\right\rangle = \sum_{i=1}^{n} T_{ij}\left|e_i\right\rangle \qquad\qquad j = 1, 2, \ldots$$

Consider a vector $\left|\alpha\right\rangle$.

$$\hat{T}\left|\alpha\right\rangle = \hat{T}\sum_{j=1}^{n} a_j\left|e_j\right\rangle$$

$$= \sum_{j=1}^{n}\sum_{i=1}^{n} a_j T_{ij}\left|e_i\right\rangle$$

we can exchange the summations, and make it look more suggestive:

$$\sum_{i=1}^{n}\left(\sum_{j=1}^{n} a_j T_{ij}\right)\left|e_i\right\rangle$$

So $\hat{T}$ transforms a vector with components $a_1, a_2, \ldots$ into a vector with components

$$a_i' = \sum_{j=1}^{n} a_j T_{ij}$$

- With an orthonormal basis,
$$T_{ij} = \left\langle e_i\right|\hat{T}\left|e_j\right\rangle$$
- A transformation is hermitian iff $\hat{T}^\dagger = \hat{T}$ if it is invariant under hermitian conjugation (conjugate transpose)
- Assuming an orthonormal basis, $\langle\alpha|\beta\rangle = \underline{a}^\dagger\underline{b}$, where $\underline{a}$ and $\underline{b}$ are column vectors
- Anti-hermitian/skew-hermitian operator: $\hat{T}^\dagger = -\hat{T}$
- $\left(\hat{A}\hat{B}\ldots\hat{Z}\right)^\dagger = \hat{Z}^\dagger\ldots\hat{B}^\dagger\hat{A}^\dagger$
- Matrix transpose: $\underline{T} \mapsto \widetilde{\underline{T}}$

If $\underline{A}$ is an unitary matrix, then

- $\underline{A}\underline{A}^\dagger = \underline{A}^\dagger\underline{A} = I \implies \underline{A}^\dagger = \underline{A}^{-1}$
- Columns of $\underline{A}$ are orthonormal
- Rows of $\underline{A}$ are orthonormal
- $\|\underline{A}\|_2 = 1$

The inverse of $\underline{A}$ only exists if $\det(\underline{A}) \neq 0$.

The determinant of any diagonal square matrix is the product of its diagonal entires.

Changing basis

A change of basis can be represented by a linear transformation. We can expand old basis vectors in terms of new ones:

$$\left|e_j\right\rangle = \sum_{i=1}^{n} S_{ij}\left|f_i\right\rangle$$

Eigenvectors and eigenvalues

The collection of all eigenvalues of a matrix is its *spectrum*.

The spectrum is degenerate when two ore more linearly independent eigenvectors share the smae eigenvalue.

Diagonalizability

$\underline{A}$ is **diagonalizable** if there exists an invertible matrix $\underline{P}$ and a diagonal matrix $\underline{D}$ such that $\underline{A} = \underline{P}\underline{D}\underline{P}^{-1}$.

$\underline{A}$ is **diagonalizable** if the columns of $\underline{P}$ are eigenvectors and the diagonal entries of $\underline{D}$ are the corresponding eigenvalues of $\underline{A}$, where $\underline{A} = \underline{P}\underline{D}\underline{P}^{-1}$.

The multiplicity of an eigenvalue is the number of times it appears as a root to the characteristic polynomial.

If a square matrix $\underline{A}$ has distinct eigenvalues (all eigenvalues have multiplicity 1), then $\underline{A}$ is diagonalizable.

A square matrix $\underline{A}$ is diagonalizable iff every eigenvalue λ of multiplicity m yields m basic eigenvectors.

(Every eigenvalue of algebraic multiplicity of m also has m geometric multiplicity. So some matrices with repeated eigenvalues are also diagonalizable.)

All *normal* matrices are diagonalizable. A matrix is normal when it commutes with its hermitian conjugate:

$$\left[\underline{A}^\dagger, \underline{A}\right] = 0$$

Always diagonalizable:

- Matrices with a basis of eigenvectors
- Matrices with distinct eigenvalues
- Hermitian matrices
- Non-zero orthogonal projection matrices

Sometimes diagonalizable:

- Matrices with repeated eigenvalues

Applications of diagonalization

Suppose $\underline{A} = \underline{P}\underline{D}\underline{P}^{-1}$.

1. Recall two properties of the determinant:
$$\det(\underline{B}\underline{C}) = \det(\underline{B})\det(\underline{C})$$
$$\det\left(\underline{B}^{-1}\right) = 1/\det(\underline{B})$$
Then,
$$\det(\underline{A}) = \det(\underline{P})\det(\underline{D})\det\left(\underline{P}^{-1}\right) = \det(\underline{D})$$
so the determinant of a diagonalizable matrix is the product of its eigenvalues
2. The trace of a square matrix is the sum of its entries on the main diagonal. We have the following property
$$\mathrm{tr}(\underline{A}\underline{B}) = \mathrm{tr}(\underline{B}\underline{A})$$
Therefore,
$$\mathrm{tr}(\underline{A}) = \mathrm{tr}(\underline{P}\underline{D}\underline{P}^{-1}) = \mathrm{tr}(\underline{P}\underline{P}^{-1}\underline{D}) = \mathrm{tr}(\underline{D})$$
So the trace of a diagonalizable matrix is the sum of its eigenvalues
3. The k^{th} power of a diagonalizable matrix, for $k \leq 0$, can be computed by
$$\underline{A}^k = \underline{P}\underline{D}^k\underline{P}^{-1}$$
If all eigenvalues of $\underline{A}$ are non-zero, then
$$\underline{D}^k = \begin{bmatrix} \lambda_1^k & 0 & & 0 \\ 0 & \lambda_2^k & & 0 \\ & & \ddots & \\ 0 & 0 & & \lambda_n^k \end{bmatrix}$$
$\forall\, k \in \mathbb{Z}$.

In general, even for non-diagonalizable matrices,

$$\det\left(\underline{A}\right) = \lambda\ldots\lambda_n$$
$$\mathrm{tr}\left(\underline{A}\right) = \lambda_1 + \cdots + \lambda_n$$

Hermitian transformations

Properties:

1. Eigenvalues of a hermitian transformation are real
2. Eigenvectors a hermitian transformation belonging to distinct eigenvalues are orthogonal
3. Eigenvectors of a hermitian transformation form an eigenbasis

Spectral theorem: Let $\underline{A}$ be a Hermitian matrix. There exists an unitary matrix $\underline{P}$ and diagonal matrix $\underline{D}$ such that

$$\underline{A} = \underline{P}\underline{D}\underline{P}^{\dagger}$$

and $\underline{A}$ is diagonalizable ("orthogonally diagonalizable").

The columns of $\underline{P}$ are a set of orthonormal eigenvectors, and the diagonal entries of $\underline{D}$ are the eigenvalues.

Leibniz's rule

Recall the following rules. For $a, b \in \mathbb{R}$, and $f(x) = dF(x)/dx$, we have

$$I = \int_a^b f(t)\,dt = F(a) - f(b)$$

Clearly,

$$\frac{d}{dx} I = 0$$

since we are differentiating a number.

Consider now

$$I = \int_a^x f(t)\,dt = F(x) - F(a)$$

If we differentiate w.r.t. x, we get

$$\frac{d}{dx} I = \underbrace{\frac{d}{dx} F(x)}_{=f(x)} - 0$$

Similarly,

$$\frac{d}{dx} \int_x^b f(t)\,dt = -f(x)$$

Let's now go to a more general case. Consider integration of f over functions v and u of x.

$$I(u, v) = \int_{u(x)}^{v(x)} f(t)\,dt$$

I should have no terms that "explicitly" depend on x alone.

By the chain rule,

$$\frac{dI}{dx} = \frac{\partial I}{\partial u}\frac{du}{dx} + \frac{\partial I}{\partial v}\frac{dv}{dx}$$

This gets us to

$$\frac{d}{dx} \int_{u(x)}^{v(x)} f(t)\,dt = f(v)\frac{dv}{dx} - f(u)\frac{du}{dx}$$

Consider the following equality:

$$\frac{d}{dx} \int_a^b f(x,t)\,dt = \int_a^b \frac{\partial f(x,t)}{\partial x}\,dt$$

the equality holds when both integrals exists.

Consider functions $f(x,t), v(x), u(x)$. *Leibniz's rule* gives a formula to the total derivative of an definite integral:

$$\frac{d}{dx} \int_{u(x)}^{v(x)} f(x,t)\,dt = f(x,v)\frac{dv}{dx} - f(x,u)\frac{du}{dx} + \int_u^v \frac{\partial f}{\partial x}\,dt$$

The rule holds when both integrals in the relation exist.

The Leibniz rule give us a nice way to evaluate some integrals.

- We know
$$I(b) = \int_0^\infty e^{-bx}\,dx = \frac{1}{b}$$
Differentiating both sides by b give
$$\frac{d^n}{db^n} \int_0^\infty e^{-bx}\,dx = \int_0^\infty \frac{\partial^n}{\partial b^n} e^{-bx}\,dx$$
$$= \int_0^\infty (-x)^n e^{-bx}\,dx = \frac{d^n}{db^n}\frac{1}{b}$$
- We know
$$I = \int_{-\infty}^\infty e^{-ax^2}\,dx = \sqrt{\frac{\pi}{a}}$$
Differentiating both sides by a.

The wave function

The Schrodinger equation

In classical mechanics, given approprate initial and boundary conditions, we can completely determine the behaviour of a conservative system using Newton's laws.

Given initial conditions ($\Psi(x,0)$) the Schrodinger equations determines the wave function $\Psi(x,t)$ for all future times

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

where $\hbar = h/2\pi = 1.054 \times 10^{-34}$ Joule-seconds.

Fundamental laws in physics are postulated. Newton nor Schrodinger derived their equations.

- $\hbar$ is also called a coupling constant.

The statistical interpretation

The wave function is a complex object that spreads out through all of space.

Born's statistical interpretation:

$$\int_a^b |\Psi(x,t)|^2\,dx$$

is the probability of finding the particle between a and b at time t. This is the integral of the complex modulus squared for Ψ.

Quantum mechanics offers statistical information about the possible results. It does not predict with certainty.

If we make a measurement, and finds the particle at a point C, where was the particle just before the measurement was made?

Realist: particles do not have an indeterminant position. And quantum mechanics is an incomplete theory. There is some additional information missing.

Orthodox (Copenhagen): the act of measurement compels the particle to take on a definite position. We do not ask why it does so (this is the measurement problem).

Agnostic: refuse the answer. It does not make sense to worry about what happens before the measurement was made, since this cannot be tested.

The current agreed upon interpretation is the orthodox position.

Making a measurement *collapases* the wave function to a sharp peak about a point. It then relaxes again. Fast repeated measurements yield similar results.

Probability

Discrete Variables

Given outcomes j, a discrete variable, $N : \mathbb{Z} \to \mathbb{Z}$, gives $N(j)$, a measure of likelihood for each possible j.

- The probability of outcome j is $P(j) = N(j)/N$.

The probability for all outcome must sum to 1:

$$\sum_j P(j) = 1$$

- *Median* outcome, i, is the outcome for which $P(j > i) = P(j < i)$
- Most probable outcome is $\max_j P(j)$

The average outcome (or expectation value), is

$$\langle j \rangle = \frac{1}{N(j)}\sum_j jN(j) = \sum_j jP(j)$$

The average value of some function of j is

$$\langle f(j) \rangle = \sum_j f(j)P(j)$$

Since the average of the deviation is zero, we define average of the square of the deviation to be the measure of spread - the *variance*:

$$\sigma^2 = \left\langle (\Delta j)^2 \right\rangle,$$

where $\Delta j = j - \langle j \rangle$ is the *deviation*.

The square root of variance is the standard deviation.

Variance identity: $\sigma^2 = \langle j^2 \rangle - \langle j \rangle^2 \geq 0$

The average of the squares is greater than the square of the average. They are equal only when $\sigma = 0$, the case where the data do not spread at all.

Continuous Variables

It only makes sense speak about the probability that an outcome x lies in some interval.

The probability that a outcome lies between x and $x + dx$ is $\rho(x)\,dx$.

The probability that an outcome lies between $[a, b]$ is

$$P_{ab} = \int_a^b \rho(x)\,dx$$

where ρ is a probability density function.

We require

$$\int_{-\infty}^{\infty} \rho(x)\,dx = 1$$

The average is

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

The average of a function of x is

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

And the standard deviation:

$$\sigma^2 = \left\langle (\Delta x)^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2$$

Normalization

We require

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = \int_{-\infty}^{\infty} \Psi^*\Psi\,dx = 1,$$

where Ψ^* denotes the complex conjugate of Ψ.

If Ψ is a solution to the Schrodinger equation, then $A \in \mathbb{C}$, $A\Psi$ is also a solution. So this additional requirement is valid.

All physical solutions are square-integrable, and are normalizable.

The Schrodinger equation preserves the normalization of the wave function. This is true when the integral has no time dependence.

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = 0$$

We can derive this result by noting $|\Psi|^2 = \Psi^*\Psi$, using product rule on $\Psi^*\Psi$, substituting the Schrodinger equation.

On the assumptions that

$$\lim_{x\to\pm\infty} \Psi(x,t) = 0, \text{ and } \mathrm{Im}\{V(x)\} = 0$$

Probability current

Recall the "continuity equation" in electrodynamics.

$$-\underline{\nabla} \cdot \underline{J} = \frac{\partial \rho}{\partial t}$$

This is the statement of the conservation of charge. If we volume integrate both sides and invoke Stoke's theorem, we get that the negative current flux is equal to the rate of change in charge.

A similar parallel can be drawn in quantum mechanics by defining a "probability current".

We define the *probability current* $[1/\mathrm{s}]$ to be

$$J = \frac{i\hbar}{2m}\left(\Psi\frac{\partial \Psi^*}{\partial x} - \Psi^*\frac{\partial \Psi}{\partial x}\right)$$

We can show that

$$\frac{d}{dt}\int_a^b |\Psi|^2\,dx = J(a,t) - J(b,t)$$

$J(x,t)$ is the rate at which probability is flowing past the point x.

The conservation of probability in 1-D quantum mechanics is that statement:

$$\frac{\partial J}{\partial x} + \frac{\partial |\Psi|^2}{\partial t} = 0$$

We will see that in higher dimensions, the "continuity equation" takes on an identical form as the one we encountered in electrodynamics.

In scattering, where we have left and right plane waves on both sides of some potential,

$$\psi_{\text{left}} = Ae^{ikx} + Be^{-ikx}$$
$$\psi_{\text{right}} = Ce^{ikx} + Be^{-ikx}$$

we have $J_{\text{left}} = J_{\text{right}}$.

Momentum

The expectation value of x is

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi(x,t)|^2\,dx$$

interpreted as the average of measurements performed using *identical particles* all described by the same Ψ.

It is not the average of repeated measurements on the same particle, as the wave function collapses after initial measurement.

We postulate that $\langle v \rangle$ is equal to $d\langle x \rangle/dt$. Since $p = mv$, the expectation value of momentum, $\langle p \rangle$ is

$$\langle p \rangle = m\langle v \rangle = -i\hbar\int \Psi^*\frac{\partial \Psi}{\partial x}\,dx$$

This correspondance of $md\langle x \rangle/dt = \langle p \rangle$, along with $d\langle p \rangle/dt = -\langle dV/dt \rangle$ is also known as Ehrenfest theorem.

The expectation values appear to obey Newton's classical equations. This is only partially true. (See wiki article on why this is not the case).

Our derivation of expectation value of momentum relied on the Schrodinger equation. We can arrive at the same result using the notion of operators.

Without the notion of operators, let's compute $d\langle x \rangle/dt$.

$$\begin{aligned}\frac{d\langle x \rangle}{dt} &= \int x\frac{\partial}{\partial t}|\Psi|^2\,dx \\ &= \int x\left(\frac{\partial \Psi^*}{dt}\Psi - \Psi^*\frac{\partial \Psi}{\partial t}\right)dx\end{aligned}$$

Using the Schrodinger equation, we can convert the time derivatives into spatial derivatives:

$$= \frac{i\hbar}{2m}\int x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{dx} + \Psi\frac{\partial \Psi^*}{\partial x}\right)dx$$

Applying integration by parts, and the assumption that $\Psi \to 0$ for $x \to \pm\infty$, we recover the expectation value for the momentum of a particle in 1-D.

Operators

Operators map functions to functions. We denote operators with a hat:

$\hat{x} = x$	Position operator
$\hat{p} = -i\hbar\frac{\partial}{\partial x}$	Momentum operator
$\hat{T} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	Kinetic energy operator

Operators do not depend on time. This is why we do not differentiate x with respect to time when computing $d\langle x \rangle/dt$.

The expectation values can be found by sandwiching operators between Ψ^* and Ψ:

$$\langle x \rangle = \int \Psi^* [x] \Psi \, dx$$

and

$$\langle p \rangle = \int \Psi^* \left[-i\hbar \frac{\partial}{\partial x} \right] \Psi \, dx$$

> The expectation value of any dynamical quantity $Q(x,p)$ can be found sandwiching an operator between Ψ^* and Ψ:
>
> $$\langle Q(x,p) \rangle = \int \Psi^* \left[Q\left(x, -i\hbar \frac{\partial}{\partial x}\right) \right] \Psi \, dx$$

Properties of operators:

- Like matrices, operators can act to the left or to the right
- Operators, $\hat{a}$, $\hat{b}$, commute when $\hat{a}\hat{b} = \hat{b}\hat{a}$

A Hermitian (self-adjoint) operator is an operator whose expectation value is real.

$$\langle \hat{p} \rangle^* = \langle \hat{p} \rangle$$

- Powers of Hermitian operators are also Hermitian operators

> Position and momentum operators are Hermitian. Such that
>
> $$\hat{x}^\dagger = \hat{x}$$
> $$\hat{p}^\dagger = \hat{p}$$
>
> sup dagger represent complex conjugation.

When $\Psi = \Psi^*$ (Ψ is real), $\langle p \rangle = 0$.

$$\begin{aligned} \langle p \rangle &= \int \Psi^* \hat{p} \Psi \, dx = -i\hbar \int \Psi^* \frac{\partial \Psi}{\partial x} \, dx \\ &= 0 \end{aligned}$$

The right will have imaginary components. But since $\hat{p}$ is self-adjoint, its expectation value cannot be imaginary, so the right must be zero.

When manipulating operators, its a good practice to assign a test function for the operators to act on. We can throw the test function away afterwards.

Uncertainty principle

Waves can have a well defined wavelength, but an ill-defined position, since it is spread out.

Waves can also have a well defined position (a single bump), but an ill-defined wavelength, since there is little periodicity.

The wavelength of Ψ is related to the momentum of particle, by the de Broglie wavelength:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$

> The more precise the position measurement of a particle is, the less precise is its momentum measurement.
>
> $$\sigma_x \sigma_p \geq \hbar/2$$

Measurements on systems with Ψ that is a single localized spike will produce widely scattered momentum measurements.

Measruements on systems with Ψ that is a long sine wave will produces widely scattered position measurements.

When considering only one of σ_x or σ_p, there is no limit on how big or small it can be.

Time-independent Schrodinger equation

Stationary states

> A time-independent potential, V, allows us to use separation of variables.

We write $\Psi(x,t) = \psi(x)\phi(t)$ and substitute into the Schrodinger equation.

$$i\hbar\psi \frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\phi + V\psi\phi$$
$$i\hbar \frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$$

Setting the both sides to equal a constant E, we get two ODES:

$$\frac{d\phi}{dt} = -\frac{iE}{\hbar}\phi$$

and

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$

A single solution to the 1-D Schrodinger equation has the form $\Psi(x,t) = \psi(x)\phi(t)$, where

$$\phi(t) = \exp(-iEt/\hbar)$$

and ψ solves the time independent Schrodinger equation

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

> All normalizable solutions satisfy $E > V_{\text{min}}$

> **Stationary states:** Solutions of the form $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$ are *stationary states* since their probability density functions are time-independent
>
> $$\Psi^*\Psi = \psi^* e^{iEt/\hbar}\psi e^{-iEt/\hbar} = \psi^*\psi$$

The Hamiltonian operator

The Hamiltonian operator is a linear operator.

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \qquad \text{Hamiltonian operator}$$

we can write the write the time-independent Schrodinger equation as

$$\hat{H}\psi = E\psi$$

The total energy of a particle is the Hamiltonian (kinetic plus potential energy):

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

The Hamiltonian operator is obtained by substituting p for the momentum operator:

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

- ψ, an eigenstate of $\hat{H}$
- E is the corresponding eigenvalue

> Any expectation value for a single eigenstate cannot depend on time.

If $\hat{H}\Psi_1 = E_1\Psi_1$, and $\hat{H}\Psi_2 = E_2\Psi_2$, and $E_1 \neq E_2$, (the Hamiltonian is not "degenerate"), so both Ψ_1 and Ψ_2 are eigenstates of the Hamiltonian.

But $\Psi_1 + \Psi_2$ cannot be an eigenstate.

$$\begin{aligned} \hat{H}(\Psi_1 + \Psi_2) &= \hat{H}\Psi_1 + \hat{H}\Psi_2 \\ &= E_1\Psi_1 + E_2\Psi_2 \\ &\neq \lambda(\Psi_1 + \Psi_2) \end{aligned}$$

The expectation value of the Hamiltonian:

$$\langle H \rangle = E \underbrace{\int \psi^*\psi \, dx}_{=1} = E$$

The expecation value of the square of the Hamiltonian:

$$\left\langle H^2 \right\rangle = \int \psi^* \hat{H}^2 \psi \, dx = E^2$$

> Every eigenstate has definite energy:
>
> $$\sigma_H^2 = \left\langle H^2 \right\rangle - \langle H \rangle^2 = 0$$

$\hat{H}$ is a linear operator implies: for $c_n \in \mathbb{C}$.

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n e^{-iE_n t/\hbar}$$

is the most general solution to the 1-D Schrodinger equation. Recall the linear differential operators we defined in the study of PDEs. Their solutions took a similar form.

The time-independent Schrodinger equation yields an infinite set of solutions, each with an associated energy. By taking a linear combination of Ψ_n, we can find a solution that matches the initial condition and boundary conditions.

Each eigenstate Ψ_n is a stationary state, but a linear superposition of eigenstates do not have to be a stationary state.

Each $c_n^* c_n$ is the probability that a measurement of the energy would return E_n. So the sum of all $|c_n|^2$ must equal 1.

The infinite square well

Is characterized by the potential:

$$V(x) = \begin{cases} 0 & x \in [0,a] \\ \infty & \text{otherwise} \end{cases}$$

We require

- ψ is continuous: $\psi(0) = \psi(a) = 0$ (boundary condition)
- ψ is normalized

Let $k = \sqrt{2mE}/\hbar$. Inside the well,

$$\frac{d^2\psi}{dx^2} = -k^2\psi,$$

Has solution

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

Applying the boudary condition, We will find that $B = 0$, and that

$$ka = n\pi$$

Quantization of energy arises from applying boundary conditions.

Each ψ (normalized) inside the well has the form

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

- From $n = 1$, each ψ_n alternate between symmetric (even) and anti-symmetric (odd) functions.

  $\psi_{1,3,5,\ldots}(a-x) = \psi_{1,3,5,\ldots}(x)$ symmetric
  $\psi_{2,4,6,\ldots}(a-x) = -\psi_{2,4,6,\ldots}(x)$ anti-symmetric

  We can define a *symmetry operator*:

  $$\mathbb{P} : x \to (a-x)$$

  So that,

  $$\mathbb{P}\psi_n = (-1)^{n+1}\psi_n$$

- Energy eigenstates are orthonormal over $[0,a]$:

  $$\int_0^a \psi_m^*\psi_n(x)\,dx = \delta_{mn}$$

- For $m \neq n$, and ψ_m, ψ_n are both symmetric/anti-symmetric,

  $$\int_{a/2}^a \psi_m^*\psi_n(x)\,dx = 0$$

- The n^{th} eigenstate has $n-1$ nodes, for $n = 1, 2, \ldots$

The energy eigenvalues (the *spectrum*) are

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 = \frac{\hbar^2}{2m}k_n^2,$$

for $n = 1, 2, \ldots$.

The eigenstates form a complete basis. Any function, $f(x)$ can be expressured as a linear combination of $\psi(x)$, even if $f(0), f(a) \neq 0$.

$$f(x) = \sum_n c_n \psi_x(x)$$

$\langle\hat{H}\rangle$ does not depend on time for any superposition of states, $f(x,t)$,

$$f(x,t) = \sum_n c_n \psi_n e^{-iE_n t/\hbar}$$

and

$$\langle\hat{H}\rangle = \int f^*\hat{H}f\,dx = \sum_n |c_n|^2 E_n$$

We can show that this is true by similarly proving

$$\langle\hat{H}\rangle = \int f^*(x,0)\hat{H}f(x,0)\,dx = \sum_n |c_n|^2 E_n$$

Since the Hamiltonian is a time independent operator, it is sufficient to consider the case at time $t = 0$.

In general, orthogonality of sines:

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx = \begin{cases} 0 & n \neq m \\ L/2 & n = m \end{cases}$$

And cosines:

$$\int_0^L \cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right)dx = \begin{cases} 0 & n \neq m \\ L/2 & n = m \neq 0 \\ L & n = m = 0 \end{cases}$$

We can compute the integrals explicitly by expanding them using complex exponentials.

A set of functions $f_n(y)$ is complete over an interval if any other function over the interval can be expanded in terms of a linear combination of them:

$$f(y) = \sum_{n=1}^{\infty} C_n f_n(y)$$

A set of functions is orthogonal over Ω if the integral of the product of any two different members of the set is zero:

$$\langle f_i, f_j\rangle := \int_\Omega f_i(y)f_j(y)\,dy = 0 \qquad \text{when } i \neq j$$

The harmonic oscillator

Has the characteristic potential:

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

Recall that in classical mechanics, the elastic potential of a spring is given by

$$U(\ell) = \frac{k}{2}(\ell - \ell_0)^2$$

where k is the spring constant, with units [kg/s^2]. The angular frequency of the oscillation is given by

$$\omega = \sqrt{\frac{k}{m}}$$

which arises naturally from the solution to the Netwon's second law.

- $k = m\omega^2$ is analogous the classical spring constant [kg/s^2]

The time independent equation is then

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

Algebraic Method

The Hamiltonian operator for our equation is

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$$

This can be written using $\hat{p}$ and $\hat{x}$:

$$\hat{H} = \frac{1}{2m}\left(i\hat{p}^2 + (m\omega\hat{x})^2\right)$$

We wish to factor $\hat{H}$. If $\hat{H}$ were a polynomial equation, then

$$u^2 + v^2 = (iu + v)(-iu + v)$$

Let's introduce the ladder operators:

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega\hat{x}\right)$$

Equivalently:

$$\hat{a} = \hat{a}_- = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}$$

and

$$\hat{a}^\dagger = \hat{a}_+ = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}$$

$\hat{a}$ and $\hat{a}^\dagger$ are hermitian conjugates of each other.

Let $x_0^2 = \hbar/m\omega$ (units of length squared), and $\xi = x/x_0$, the ladder operators become

$$\hat{a} = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_0} + i\frac{x_0\hat{p}}{\hbar}\right) = \frac{1}{\sqrt{2}}\left(\hat{\xi} + \frac{\partial}{\partial\xi}\right)$$
$$\hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(\hat{\xi} - \frac{\partial}{\partial\xi}\right)$$

We can see that

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}\left(i\hat{p} + m\omega\hat{x}\right)\left(-i\hat{p} + m\omega\hat{x}\right)$$
$$= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 - im\omega\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)\right)$$

The additional term, $\hat{x}\hat{p} - \hat{p}\hat{x}$ is the *commutator* of $\hat{x}$ and $\hat{p}$.

The ordering of $\hat{a}_-$ and $\hat{a}_+$ also matters, as they do not commute.

The commutator of two operators is an operator that measures of how well two operators commute. In general the commutator of $\hat{A}$ and $\hat{B}$ is denoted

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Properties of commutators:

- Antisymmetry: $\left[\hat{A}, \hat{B}\right] = -\left[\hat{B}, \hat{A}\right]$
- Hermitian conjugation: $\left[\hat{A}, \hat{B}\right]^\dagger = \left[\hat{B}^\dagger, \hat{A}^\dagger\right]$
- Operators and constants always commute $\left[c, \hat{A}\right] = 0$
- Linearity: $\left[\hat{A}, \hat{B} + \hat{C} + \ldots\right] = \left[\hat{A}, \hat{B}\right] + \left[\hat{A}, \hat{C}\right] + \ldots$
- We can always factor coefficients in operators out of the commutator:

$$\left[a\hat{A}/b, c\hat{B}/d\right] = \frac{ac}{bd}\left[\hat{A}, \hat{B}\right]$$

- Jacobi identity:

$$\left[\hat{A}, \left[\hat{B}, \hat{C}\right]\right] + \left[\hat{B}, \left[\hat{C}, \hat{A}\right]\right] + \left[\hat{C}, \left[\hat{A}, \hat{B}\right]\right] = 0$$

The canonical commutation relation is

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

Let's compute the commutator of the position and momentum operator.

First, let $f(x)$ be a test function.

$$\hat{x}\hat{p}f - \hat{p}\hat{x}f = x(-i\hbar)\frac{\partial}{\partial x}f(x) - (-i\hbar)\frac{\partial}{\partial x}(xf)$$
$$= i\hbar f$$

Throwing f away, we find that that $[\hat{x}, \hat{p}]$ is $i\hbar$.

Mysterys of quantum mechanics can be traced back to this relation. Its sometimes taken to be an axiom of the theory.

We have:

$$\hat{a}_\pm\hat{a}_\mp = \frac{1}{\hbar\omega}\hat{H} \mp \frac{1}{2}$$

- $\hat{a}_-\hat{a}_+ = (\hat{a}_+\hat{a}_- + 1)$
- $\left[\hat{a}, \hat{a}^\dagger\right] = 1$
- $\left[\hat{a}^\dagger, \hat{a}\right] = -1$
- $\left[\hat{H}, \hat{a}\right] = -\hbar\omega\hat{a}$

  First, we use

  $$\left[\hat{A} + \hat{B}, \hat{C} + \hat{D}\right] = \left[\hat{A}, \hat{C}\right] + \left[\hat{B}, \hat{C}\right] + \left[\hat{A}, \hat{D}\right] + \left[\hat{B}, \hat{D}\right]$$

  to write

  $$\left[\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \hat{a}\right] = \hbar\omega\left[\hat{a}^\dagger\hat{a}, \hat{a}\right] + \hbar\omega\left[\frac{1}{2}, a\right]$$

  Then, we can apply

  $$\left[\hat{A}\hat{B}, \hat{C}\right] = \left[\hat{A}, \hat{C}\right]\hat{B} + \hat{A}\left[\hat{B}, \hat{C}\right]$$

  To the first term:

  $$\hbar\omega\left(\left[\hat{a}^\dagger, \hat{a}\right]\hat{a} + \hat{a}^\dagger\left[\hat{a}, \hat{a}\right]\right)$$

  Which simplifies to our desired result.
- $\left[\hat{H}, \hat{a}^\dagger\right] = \hbar\omega\hat{a}^\dagger$

Using a_- and a_+, we factor the Hamiltonian:

$$\hat{H} = \hbar\omega\left(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2}\right)$$

Equivalently:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

Rewriting the time independent equation:

$$\hbar\omega\left(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2}\right)\psi = E\psi$$

Let ψ is an normalized eigenstate of the Hamiltonian,

$$\hat{H}\psi = E\psi \quad \text{then} \quad \hat{H}\hat{a}_\pm\psi = (E \pm \hbar\omega)\,\psi$$

We introduced this result as a postulate. But here is the derivation. Consider

$$\left(\left[\hat{H}, \hat{a}^\dagger\right] - \hbar\omega\hat{a}^\dagger\right)\psi_n = 0$$

We can verify that this equality holds. Assuming we have solved the Schrodinger equation, (we have $\hat{H}\psi = E\psi$ as a relation at our disposal) we can manipulate this equation to arrive at our desired result.

We can explicitly show that $\hat{a}_\pm\psi$ is also an eigenstate of $\hat{H}$ with eigenvalue $E \pm \hbar\omega$.

$$\hat{H}a_\pm\psi = \hbar\omega\left(\hat{a}_\pm\hat{a}_\mp \pm \frac{1}{2}\right)a_\pm\psi = \hbar\omega\left(\hat{a}_\pm\hat{a}_\mp a_\pm \pm \frac{1}{2}a_\pm\right)\psi$$
$$= \hat{a}_\pm\hbar\omega\left(\hat{a}_\mp a_\pm \pm \frac{1}{2}\right)\psi = \hat{a}_\pm\hbar\omega\left(\hat{a}_\pm a_\pm \pm 1 \pm \frac{1}{2}\right)\psi$$
$$= \hat{a}_\pm\left(\hat{H} \pm \hbar\omega\right)\psi = \hat{a}_\pm E\psi \pm \hat{a}_\pm\hbar\omega\psi$$
$$= \hat{a}_\pm\left(E \pm \hbar\omega\right)\psi$$
$$= \left(E \pm \hbar\omega\right)\hat{a}_\pm\psi$$

Operators $\hat{a}_+, \hat{a}_-$ are *raising and lowering ladder operators*.

- Given an eigenstate ψ, we can find all other eigenstates by applying $\hat{a}_\pm$
- $\hat{a}_-^n\psi$ need not be normalizable, since $(E - n\hbar\omega)$ will eventually be less than V_{min}

The lowest energy state of the harmonic oscillator potential is found by setting

$$\hat{a}_- \psi_0 = 0$$

This is the **ONLY** consistent solution.

While we have started our numbering from 1 in the past, ground state starts from 0 from the harmonic oscillator.

This is a first order ODE with the solution

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(\frac{-m\omega}{2\hbar}x^2\right)$$

In terms of ξ:

$$\psi_0(\xi) = \frac{1}{x_0^{1/2}\pi^{1/4}} e^{-\xi^2/2}$$

We see that

$$\int \psi_n^\dagger \psi_n \, dx = \int \psi_n^\dagger \psi_n x_0 \, d\xi = 1$$

Thus:

$$\int \psi_n^\dagger \psi_n \, d\xi = \frac{1}{x_0}$$

To change the differentiation variable from x to ξ, we do the following:

$$\frac{\partial \psi(\xi(x))}{\partial x} = \frac{\partial \psi}{\partial \xi}\frac{\partial \xi}{\partial x}$$

which means that

$$\frac{\partial}{\partial x} \mapsto \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi}$$

For the second partial, we need to apply the product rule:

$$\begin{aligned}\frac{\partial^2 \psi}{\partial x^2} &= \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi}\left(\frac{\partial \psi}{\partial \xi}\frac{\partial \xi}{\partial x}\right) \\ &= \left(\frac{d\xi}{dx}\right)^2 \frac{d^2\psi}{d\xi^2} + \frac{d\psi}{d\xi}\frac{d^2\xi}{dx^2}\end{aligned}$$

Thus:

$$\frac{\partial^2}{\partial x^2} \mapsto \left(\frac{\partial \xi}{\partial x}\right)^2 \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2 \xi}{\partial x^2}\frac{\partial}{\partial \xi}$$

The ground state energy is $E_0 = \hbar\omega/2$. We can find this by substituting it into the time independent equation written using the Hamiltonian in terms of the ladder operators.

The n^{th} excited eigenstates of the quantum oscillator potential can be found by

$$\psi_n = A_n \hat{a}_+^n \psi_0 \qquad E_n = \hbar\omega\left(\frac{1}{2} + n\right)$$

where A_n is the n^{th} normalization constant, given by

$$A_n = \frac{1}{\sqrt{n!}}$$

We can derive the normalization constant for all eigenstates algebraically. First, let's consider

$$\hat{a}\psi_n = c_n \psi_{n-1},$$

where c_n is the normalization constant for ψ_{n-1}, and we assume that ψ_n is already nromalized.

1. Take the hermitian conjugate of both sides:

   $$\psi_n^\dagger \hat{a}^\dagger = c_n^* \psi_{n-1}^\dagger$$

   the hermitian conjugate of numbers is simply the complex conjugate.

2. Multiply conjugated expression by the original

   $$\begin{aligned}\psi_n^\dagger \hat{a}^\dagger \hat{a} \psi_n &= c_n^* \psi_{n-1}^\dagger c_n \psi_{n-1} \\ &= |c_n|^2 \psi_{n-1}^\dagger \psi_{n-1}\end{aligned}$$

3. Write $\hat{a}^\dagger\hat{a}$ in terms of the Hamiltonian:

   $$\hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}$$

4. Substitute into our expression:

   $$\psi_n^\dagger \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)\psi_n = |c_n|^2 \psi_{n-1}^\dagger \psi_{n-1}$$

5. Integrate both sides. Consider the integral on the right:

   $$|c_n|^2 \int \psi_{n-1}^\dagger \psi_{n-1} \, dx = |c_n|^2$$

   This is due to our normalization condition. Consider now the integral on the left:

   $$\begin{aligned}\int \psi_n^\dagger \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)\psi_n \, dx &= \int \psi_n^\dagger \frac{\hat{H}}{\hbar\omega}\psi_n \, dx - \frac{1}{2}\int \psi_n^\dagger \psi_n \, dx \\ &= \left(n + \frac{1}{2}\right) - \frac{1}{2} \\ &= n\end{aligned}$$

6. Equate the left and right integrals:

   $$c_n = \sqrt{n} \iff \hat{a}\psi_n = \sqrt{n}\psi_{n-1}$$

In a similar fashion, we can find that

$$\hat{a}^\dagger \psi_n = \sqrt{n+1}\psi_{n+1}$$

Assuming ψ_n is normalized:

$$\begin{aligned}\hat{a}\psi_n &= \sqrt{n}\psi_{n-1} \\ \hat{a}^\dagger\psi_n &= \sqrt{n+1}\psi_{n+1}\end{aligned}$$

Different stationary states of the same Hamiltonian are orthogonal.

$$\int \psi_m^\dagger \psi_n \, dx = \delta_{mn}$$

We can use an operators approach to when integrating ψ_m and ψ_n. The key is to utilize the identity:

$$\hat{a}\psi_0 = 0$$

and its hermitian conjugate:

$$\psi_0^\dagger \hat{a}^\dagger = 0$$

and the fact that any excited state can be found be repeated applying the raising operator to the ground state.

In position space, we can express the position and momentum operator in terms of $\hat{a}, \hat{a}^\dagger$.

$$\begin{aligned}\hat{x} &= \frac{x_0}{\sqrt{2}}\left(\hat{a}^\dagger + \hat{a}\right) \\ \hat{p} &= \frac{i\hbar}{x_0\sqrt{2}}\left(\hat{a}^\dagger - \hat{a}\right)\end{aligned}$$

Instead of directly computing $\langle\psi_n|\,\hat{x}\,|\psi_m\rangle$, we can leverage orthogoality by writing $\hat{x}$ using $\hat{a}, \hat{a}^\dagger$.

First three eigenstates:

$$\begin{aligned}\psi_0 &= \alpha e^{-\xi^2/2} \\ \psi_1 &= \sqrt{2}\alpha\xi e^{-\xi^2/2} \\ \psi_2 &= \frac{\alpha}{\sqrt{2}}\left(2\xi^2 - 1\right)e^{-\xi^2/2}\end{aligned}$$

where $\alpha = 1/(x_0^{1/2}\pi^{1/4})$, $x_0^2 = \hbar/m\omega$, $\xi = x/x_0$.

The free particle

The free particle is characterized by

$$V(x) = 0 \qquad \forall x \in \Omega$$

Recall that the time-independent equation can be put into the form

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

where $k = \sqrt{2mE}/\hbar$.

The solution has the form

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

which can be converted interms of sines and cosines.

The general solution to the time-dependent equation is

$$\Psi(x,t) = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)} + Be^{-ik\left(x + \frac{\hbar k}{2m}t\right)}$$

Functions of the form $f(x \pm vt)$ are waves travelling to the $\mp x$ direction with speed v.

Every point in the wave travels with the same speed v, and the shape of wave remains the same as it travels.

Letting $k = \pm\sqrt{2mE}/\hbar$, we can write

$$\Psi_k = Ae^{ik\left(x - \frac{\hbar k}{2m}t\right)} = Ae^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}$$

and $\pm k$ corresponds to waves traveling in $\pm x$ direction (called *plane wave solutions*).

We can expand

$$e^{ik\left(x-\frac{\hbar k}{2m}t\right)} = e^{ikx}e^{-ik\frac{\hbar k}{2m}t}$$

Recall that

$$e^{i\theta} = e^{i\theta+i2\pi n} = e^{i\theta}e^{i2\pi n} = e^{i\theta}$$

Thus

$$e^{ikx} = e^{ikx+i2\pi n} = e^{ikx}e^{i2\pi n}$$

this means for every multiple of $2\pi/k$, the wave repeats it self. This means that Ψ has wave length

$$\lambda = 2\pi/|k|$$

This is analogous to the classical mechanical wave equation:

$$y(x,t) = A\sin(kx-\omega t+\phi)$$

where k is the wave number, such that $k = 2\pi/\lambda$, $\omega = 2\pi/T$, and ϕ is the phase.

- k plays same the role of the wave number in a classical plane wave
- $\hbar k^2/2m$ plays the role of angular frequency, $\hbar k^2/2m = 2\pi f$

The plane wave solutions have a well defined momentum, given by de Broglie:

$$p = \frac{2\pi\hbar}{\lambda} = \hbar k$$

Wave functions with a definite momentum are eigenstates of the momentum operator:

$$\hat{p}\Psi_k = \hbar k\Psi_k$$

A superposition of states are not necessarily eigenstates.

Since $v = \lambda f$,

$$v_{\text{quantum}} = \frac{2\pi}{k}\frac{\hbar k^2}{4\pi m} = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$$

Recall that classical kinetic energy is

$$E = \frac{1}{2}mv^2 \implies v = \sqrt{\frac{2E}{m}}$$

The wave function travels half as fast as the particle it represents.

The separable solution (plane wave solution) to the Schrodinger equation is not normalizable.

$$\int_{-\infty}^{\infty}\Psi_k^*\Psi_k\,dx = |A|^2\int_{-\infty}^{\infty}dx = |A|^2(\infty)$$

- A free particle cannot exist in a stationary state
- Plane waves cannot represent free particles

Instead of summing over and index, we integrate over k (hence a range of energies and speeds), to find a general solution to the time-dependent equation. This is the wave packet solution:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}\,dk$$

$\phi(k)/\sqrt{2\pi}\,dk$ plays the role of c_n.

The equation must satisfy our initial condition:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ikx}\,dk$$

We recognize that this is the INVCTFT of $\phi(k)$. To find $\phi(k)$, we find the CTFT of $\Psi(x,0)$:

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)e^{-ikx}\,dx$$

Parseval's Theorem for CTFT: the normalized wave function in real space remain normalized in momentum space

$$\int_{-\infty}^{\infty}|\Psi(x,0)|^2\,dx = \int_{-\infty}^{\infty}|g(k)|^2\,dk$$

We are transforming between position and k-space. Since $p = \hbar k$, we can also say that we can transforming between momentum and position space.

Also, this definition of CTFT has a different normalization constant than what we encountered in other courses.

There is another interpretation to this normalization. We are normalizing to the delta function:

$$\int\Psi_p^*(x)\Psi_{p'}(x)\,dx = \delta(p-p')$$

$\phi(k)\,dk$ is the probability to find a particle with momentum between $\hbar k$ and $\hbar(k+dk)$.

Instead of transforming into k-space, we can transform into momentum-space instead.

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\phi(p)e^{ipx/\hbar}\,dp$$

and

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

Since if

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

we have

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\,dp = \delta(x)$$

The delta function potential

Bound and scattering states

We have seen two types of general solutions to the Schrodinger equation.

1. Sum of eigenstates over an index: infinite well
2. Integral of eigenstates over wave number k: free particle

In classical mechanics, we have the distinction of bound and scattering states.

We have a bound state when the energy of the particle is less than that of the potential, and the particle cannot escape.

In a scattering state, the particle energy is more than that of the potential.

We say an eigenstate is a scattering or bound state by the following criterion:

$$\begin{cases} E < V(-\infty)\wedge V(+\infty) & \text{bound} \\ E > V(-\infty)\wedge V(+\infty) & \text{scattering} \end{cases}$$

The delta function potential support both bound and scattering states.

- Bound states are differentiated by an discrete index
- Scattering states are differentiated by a continuous variable

If V goes to zero for $x\to\infty$, then E alone determines whether we have a bound or scattering state.

So the free particle potential ($V = 0$ every where) result in only scattering states, and the square well result in only bound states.

Recall the general rule, that we require $E > V_{\min}$, but this does not apply as the scattering states are not normalizable in the way we do for bound states.

The delta-function well

The characteristic potential is:

$$V(x) = -\alpha\delta(x),$$

where $\alpha\in\mathbb{R}$, and

$$\delta(x) = \begin{cases} 0 & x\neq 0 \\ \infty & x = 0 \end{cases}$$

- The delta function has units [1/Length]
- α has units [Energy/Length]

Bound states ($E < 0$): When $x \neq 0$, the time independent Schrodinger equation reads

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

If we divide both sides by $-\hbar^2/2m$.Since $E < 0$, κ be real and positive:

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

Our time independent eqution becomes:

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

The general solution to

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

To determine the constants, we require the following conditions:

1. ψ is symmetric
2. ψ is continuous
3. $d\psi/dx$ is continuous except where V is infinite
4. $\psi \to 0$ when $x \to \pm\infty$

The general solution to the time independent equation is

$$\psi(x) = \begin{cases} Be^{-\kappa x} & x \geq 0 \\ Be^{\kappa x} & x \leq 0 \end{cases}$$

The delta function adds a discontinuity to $d\psi/dx$. It modifies the boundary condition at $x = 0$ from $\Delta(d\psi/dx) = 0$ to :

$$\lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}(\epsilon) - \frac{d\psi}{dx}(-\epsilon)\right) = \frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon} V\psi\, dx$$

If we integrate the time independent equation over $[-\epsilon, \epsilon]$,

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}\,dx + \int_{-\epsilon}^{\epsilon} V\psi\, dx = E\int_{-\epsilon}^{\epsilon}\psi\, dx$$

In the limit as $\epsilon \to 0$, the leftmost term becomes

$$-\frac{\hbar^2}{2m}\left(\frac{d\psi}{dx}(\epsilon) - \frac{d\psi}{dx}(-\epsilon)\right)$$

The rightmost term must be zero. Rearranging,

$$\left(\frac{d\psi}{dx}(\epsilon) - \frac{d\psi}{dx}(-\epsilon)\right) = \frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon} V\psi\, dx$$

When V is finite, the right hand side is zero. Since the difference between the derivative of ψ at two infinitely close neighbouring points is zero, we conclude that ψ is continuous.

For $V = -\alpha\delta(x)$, we have

$$\Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

This leads to

$$\kappa = \frac{m\alpha}{\hbar^2}$$

which result in

$$E = \frac{-\hbar^2\kappa^2}{2m}$$

The delta function potential only admits a single energy level

Normalizing ψ gives $B = \sqrt{\kappa}$, and the general solution becomes

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\exp\left(\frac{-m\alpha|x|}{\hbar^2}\right)$$

Scattering states ($E > 0$): Since $E < 0$, we define k

$$k = \frac{\sqrt{2mE}}{\hbar}$$

and the time independent equation is

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

The general solution are is similar to what we found for the free particle.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Fe^{ikx} + Ge^{ikx} & x > 0 \end{cases}$$

Applying

1. Continuity at 0 gives:

$$A + B = F + G$$

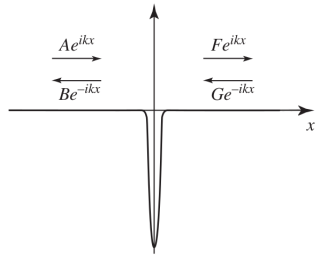
2. Discontinuity condition at $x = 0$:

$$ik(F - G - A + B) = \frac{-2m\alpha}{\hbar^2}(A + B)$$

defining $\beta = \frac{m\alpha}{\hbar^2 k}$, we can write

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta)$$

When we consider the time dependent term, from the free particle case we know that our solution resemble plane waves.



Interpreting A, B, G, F as amplitudes:

- A: wave coming from the left
- G: wave coming from the right
- B: wave return to the left
- F wave travelling off to the right

we can set any one of A, B, G, F to zero, and interpret the remain coefficients as terms describing an incident wave, reflected wave, and trasmitted wave across the delta potential.

$$G = 0$$

let's us say that

- A: incident wave
- F: transmitted wave
- B: reflected wave

We can arrange

$$A + B = F + G$$

and

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta)$$

to write B and F in terms of A.

$$B = \frac{i\beta}{1 - i\beta}A$$

and

$$F = \frac{1}{1 - i\beta}A$$

Reflection coefficient: The relative probability that an incident particle will be reflected back:

$$R = \left|\frac{J_{\text{reflected}}}{J_{\text{incident}}}\right|$$

Transmission coefficient: The relative probability that a particle will travel through the potential:

$$T = \left| \frac{J_{\text{transmitted}}}{J_{\text{incident}}} \right|$$

In our case:

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} \qquad \beta = \frac{m\alpha}{\hbar^2 k}$$
$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}$$

- $R + T = 1$
- R and T are independent of α (sign of V), so a quantum particle is just as likely to pass through a barrier as to cross over a well

We could have written the out-going amplitudes, B and F, as a function of the in-going amplitudes, A and G:

$$B = S_{11}A + S_{12}G$$
$$F = S_{21}A + S_{22}G$$

We define the **S-matrix**, or **Scattering matrix** as the matrix that relates B, F to A, G:

$$\begin{bmatrix} B \\ F \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} A \\ G \end{bmatrix}$$

In our case,

$$\underline{\underline{S}} = \frac{1}{1-i\beta} \begin{bmatrix} i\beta & 1 \\ 1 & i\beta \end{bmatrix}$$

$\underline{\underline{S}}$ is unitary (but not hermitian):

$$\underline{\underline{S}}^\dagger \underline{\underline{S}} = \underline{\underline{I}}$$

Notice that each term in ψ, if we interpret it as a superposition of left and right travelling waves, is not normalizable.

We know how to deal with it, but integrating over k, and thereby a range of energies, as we did for the free particle.

Only when we get a wave packet is our solution normalizable.

"R and T should be interpreted as the approximate relfection and transmission probabilities for particles with energies in the vicinity of E"

The fact that T is non zero, even for an infinitely deep/tall delta well/barrier, is the phenomenon of quantum tunnelling.

Dirac Delta

We can define it in two ways:

1. $\delta(x)$ as a limit of a sequence fo functions peaked at $x = 0$. In the limit, the peak rises and the width shrinks in such a way that the area under the curve remains 1.

   $$\delta(x) = \lim_{\epsilon \to 0} \delta_\epsilon(x)$$

   where

   $$\delta_\epsilon(x) = \begin{cases} \frac{1}{\epsilon} & -\epsilon/2 < x < \epsilon/2 \\ 0 & \text{otherwise} \end{cases}$$

   Similarly,

   $$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{\pi} \frac{\epsilon}{\epsilon^2 + x^2}$$

   (In the limit as ϵ goes to zero, but never zero.)

2. For some $\epsilon > 0, \epsilon \in \mathbb{R}$,

   $$\int_{a-\epsilon}^{a+\epsilon} f(x)\delta(x-a)\,dx = f(a)$$

Equivalence

Expressions $D_1(x), D_2(x)$ involving the delta function are equal if

$$\int_{-\infty}^{\infty} f(x)D_1(x)\,dx = \int_{-\infty}^{\infty} f(x)D_2(x)\,dx,$$

for all $f(x)$.

Scaling

$$\delta(kx) = \delta(x)/|k|$$

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

Three dimensions

$$\delta^3(\underline{r}) = \prod_{i=1}^{3} \delta(x_i)$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\underline{r})\delta^3(\underline{r} - \underline{a})\,dV = f(\underline{a})$$

Differentiation

By repeated applications of integration by parts, we can show that

$$\int_{-\infty}^{\infty} f(x)\frac{d^n}{dx^n}\delta(x-a)\,dx = (-1)^n \frac{d^n f}{dx^n}(a)$$

We can also think of $\delta(x)$ as

$$\delta(x) = \frac{d}{dx}\theta(x)$$

where $\theta(x)$ is the step function.

Formalism

Hilbert Space

Quantum theory is based on wave functions and operator.

Wave functions: represent the state of a system

Operators: represent observables.

Operators act on wave functions as linear transformations.

The space of all square integrable functions defined over a domain Ω, is an instance of a more general abstract vector space, called a *Hilbert space*. L^2 is only an example of a Hilbert space.

$$f \in L^2(\Omega) \iff \int_\Omega |f|^2\,dx < 0$$

All wave functions live in L^2.

The inner product of two functions, $f(x), g(x) \in L^2(a,b)$ is given by:

$$\langle f|g\rangle = \int_a^b f^*(x)g(x)\,dx$$

When $f, g \in L^2$, their inner product must exist. This comes from the integral Schwarz inequality:

$$\left|\int_a^b f^*(x)g(x)\,dx\right| \le \sqrt{\int_a^b |f(x)|^2\,dx \int_a^b |g(x)|^2\,dx}$$

Properties of the L^2 inner product:

- Non-commutative: $\langle g|f\rangle = \langle f|g\rangle^*$
- $\langle f|f\rangle \ge 0$; $\langle f|f\rangle = 0 \iff f = 0$

Schwarz inequality: $|\langle f|g\rangle|^2 \le \langle f|f\rangle \langle g|g\rangle$

In linear algebra, we are more familiar with the following statement:

$$|\underline{v} \cdot \underline{w}| \le \|\underline{v}\|\|\underline{w}\|$$

A set of functions, V, is:

- orthonormal when any $f_m, f_n \in V$:

  $$\langle f_m|f_n\rangle = \delta_{mn}$$

- complete when any other L^2 function $g(x)$ can be expanded in terms of functions of V:

  $$g(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

- When V is an orthonormal set,

  $$c_n = \langle f_n|g\rangle$$

Observables

Hermitian operators represent observables, since the expectation value of hermitian operators is real.

The expectation value of an observables is can be written as

$$\langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle = \langle Q \rangle^*$$

The expectation value is real, so it is equal to its complex conjugate.Recall the adjoint of $\hat{Q}$, $\hat{Q}^\dagger$ has the property that

$$\langle f | \hat{Q} g \rangle = \left\langle \hat{Q}^\dagger f \middle| g \right\rangle$$

All hermitian (self-adjoint) operators satisfy:

- $\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle$
- $\hat{Q} = \hat{Q}^\dagger$

An operator that is hermitian on the real line may not be hermitian on a finite interval.

Determinate states

A determinate state, Ψ, for an observable, Q, is such that every measurement of Q on Ψ returns the same value. For example, a single eigenstate of the Hamiltonian is a determinate state of energy. Every measurement of energy on a systems of that eigenstate will return a single energy value.

Since σ_Q^2 must be zero for determinate states:

$$\sigma_Q^2 = \left\langle (Q - \langle Q \rangle)^2 \right\rangle = 0$$

This is the expectation value of the deviation squared:

$$\left\langle \Psi \middle| (\hat{Q} - \langle Q \rangle)^2 \Psi \right\rangle$$

Since $\hat{Q}$ is hermitian, so too is $\hat{Q} - \langle Q \rangle$. This lets us move a factor of deviation over:

$$\langle (\hat{Q} - \langle Q \rangle)\Psi | (\hat{Q} - \langle Q \rangle)\Psi \rangle = 0$$

The only vector whose inner product with it self vanishes is $|0\rangle$. We can conclude:

All determinate states of Q are eigenfunctions of $\hat{Q}$

$$\hat{Q}\Psi = q\Psi$$

- The set of all eigenvalues of a operator is the *spectrum* of the operator
- The spectrum is degenerate when two linearly independen eigenfunctions share the same eigenvalue

Eigenfunctions of a hermitian operator

When the spectrum is discrete:

- Eigenfunctions are in Hilbert space (thus normalizable)
- They are physically realizable states

Whent the spectrum is continuous:

- Eigenfunctions are not normalizable
- A superposition of eigenfunctions may be normalizable
- On their own, they are not physically realizable

Discrete spectra

Eigenvalues of normalizable eigenfunctions of a Hermitian operator are real.

Eigenfunctions of distinct eigenvalues are orthogonal.

Its possible to use Gram-Schmidt to construct a orthonormal basis of eigenfunctions.

In a finite dimensional vector space, eigenvectors of a Hermitian matrix form an eigenbasis.

Eigenfunctions of an observable operator are complete: Any function (in Hilbert space) can be expressed as a linear combination of them.

Continuous Spectra

Eigenvalues of the hermitian operators are labeled by a continuous variable.

- Eigenfunctions are not normalizable, ($\notin H(\Omega)$)
- Eigenfunctions with real eigenvalues are *Dirac orthonormalizable* and complete

Momentum operator: Consider the eigenvalue problem involving the 1-D momentum operator.

$$-i\hbar \frac{d}{dx} f_p(x) = p f_p(x)$$

This is a 1-D separable ODE we can solve:

$$f_p(x) = A e^{ipx/\hbar}$$

$f_p(x) \notin H(\Omega)$, but if we only consider eigenvalues $p \in \mathbb{R}$, then

$$\left\langle f_{p'} \middle| f_p \right\rangle = |A|^2 \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\, dx$$

By a fourier transform identity, and letting $A = 1/\sqrt{2\pi\hbar}$ we arrive at

$$\left\langle f_{p'} \middle| f_p \right\rangle = \delta(p - p')$$

The eigenfunctions of the momentum operator

$$f_p = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

are sinusoidal, with wavelength equal to the de Broglie wavelength, $2\pi\hbar/p$.

Position operator: The eigenvalue problem:

$$\hat{x} g_y(x) = x g_y(x) = y g_y(x)$$

The only function such that multiplying by a variable is the same as multiplication a constant y is the Dirac delta. When $g_{y'} = A\delta(x - y')$, $A = 1$, we can check that

$$\left\langle g_{y'} \middle| g_y \right\rangle = \delta(y - y')$$

Generalized statistical interpretation

Generalized statiscal interpretation: Consider a particle in a general state $\Psi(x,t)$. A measurement of an observable $Q(x,p)$ will return an eigenvalue of the hermitian operator

$$\hat{Q}(\hat{x}, \hat{p})$$

When the spectrum is discrete, then the probability of getting eigenvalue q_n associated with the orthonormal eigenfunction $f_n(x)$ is

$$|c_n|^2 \qquad c_n = \langle f_n | \Psi \rangle$$

When the spectrum is continuous, the probility of getting $q(z)$ associated with the Dirac-orthonormal eigenfunction $f_z(x)$, within dz, is

$$|c(z)|^2\, dz \qquad c(z) = \langle f_z | \Psi \rangle$$

The wave function collapses into the eigenstate upon measurement.

The uncertainty principle

Proof of the generalized uncertainty principle

Consider two hermitian operators, $\hat{A}$ and $\hat{B}$. Let us define,

$$\Delta\hat{A} = \hat{A} - \langle A\rangle$$
$$\Delta\hat{B} = \hat{B} - \langle B\rangle$$

and

$$f = \Delta\hat{A}\Psi$$
$$g = \Delta\hat{B}\Psi$$

Since $\hat{A}$ and $\hat{B}$ are hermitian, we have

$$\sigma_A^2 = \langle f|f\rangle$$

and

$$\sigma_B^2 = \langle g|g\rangle$$

The product of σ_A^2 and σ_B^2 is the upper bound of $|\langle f|g\rangle|^2$, by the Schwarz inequality.:

$$\langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2$$

Since $|z|^2 \geq \mathrm{Im}(z)^2$ for all $z \in \mathbb{C}$, we have

$$|\langle f|g\rangle|^2 \geq \left(\frac{\langle f|g\rangle - \langle g|f\rangle}{2i}\right)^2$$

Let's consider the terms $\langle f|g\rangle$ and $\langle g|f\rangle$. Since $\Delta\hat{A}$ and $\hat{B}$ are hermitian, we can write

$$\langle f|g\rangle = \langle\Psi|\Delta\hat{A}\Delta\hat{B}\Psi\rangle$$

We can expand $\Delta\hat{A}\Delta\hat{B}$:

$$\hat{A}\hat{B} - \hat{A}\langle B\rangle - \langle A\rangle\hat{B} + \langle A\rangle\langle A\rangle$$

This lets us break up $\langle\Psi|\Delta\hat{A}\Delta\hat{B}\Psi\rangle$ into a sum of inner products.

$$\langle\Psi|\Delta\hat{A}\Delta\hat{B}\Psi\rangle = \langle\Psi|\hat{A}\hat{B}\Psi\rangle - \langle B\rangle\langle\Psi|\hat{A}\Psi\rangle - \langle A\rangle\langle\Psi|\hat{B}\Psi\rangle + \langle A\rangle\langle B\rangle\langle\Psi|\Psi\rangle$$

We can show that

$$\langle f|g\rangle = \langle\hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$$
$$\langle g|f\rangle = \langle\hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle$$

Then,

$$\langle f|g\rangle - \langle g|f\rangle = \langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle = \langle[\hat{A},\hat{B}]\rangle$$

Given two hermitian operators, $\hat{A}$ and $\hat{B}$, we have

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2$$

When the operators commutute, $\sigma_A\sigma_B \geq 0$

The commutator of two hermitian operators is *anti-hermitian*, such that

$$\hat{Q}^\dagger = -\hat{Q}$$

When two hermitian operators commute, their observables are said to be *compatible*. Compatible observables:

- share a complete set of eigenfunctions
- we can measure both observables at the same time

When two hermitian operators do not commute, their observables are said to be *incompatible*. Incompatible observables:

- do not share a complete set of eigenfunctions
- measuring one observable will render the measurement of other observable obsolete

For example, measuring the position of the particle collapses the wave function to an eigenstate of the position operator (a delta function). The fourier transform into momentum space will be a complex exponential.

Measuing the momentum of the particle collapses the wave function into an eigenstate of the momentum operator (a complex exponential). And its position will be undefined.

The minimum-uncertainty wave packet

The energy-time uncertainty principle

Vectors and Operators

Bases in Hilbert Space

- The physical state of a system is represented by a state vector that lives in Hilbert space
- We can choose the basis we want to represent them in
- Operators are transformations on Hilbert space - they transform once vector into another
- While $\Psi(x,t)$ represents a quantum state in the *position basis*, $\Phi(x,t)$ is an equal representatopm in *momentum basis*

Let $|x\rangle$ denote eigenfunctions of $\hat{x}$ with eigenvalue x, $|p\rangle$ be eigenfunctions of $\hat{p}$ with eigenvalue p, and $|S(t)\rangle$ be a general quantum state. Then

$$\Psi(x,t) = \langle x|S(t)\rangle$$
$$\Phi(p,t) = \langle p|S(t)\rangle$$

We do not specify the form of $\hat{x}$ or $\hat{p}$. Since their representations also depend on what basis we express them in.

A vector can be expanded in terms of an orthonormal basis:

$$|\alpha\rangle = \sum_n a_n|e_n\rangle \iff a_n = \langle e_n|\alpha\rangle$$

An operator in a particular basis are represented by their *matrix element* (often an infinite number of them),

$$\langle e_m|\hat{Q}|e_n\rangle = Q_{mn}$$

Consider the following transformation:

$$|\beta\rangle = \hat{Q}|\alpha\rangle$$

In a particular basis, we have

$$\sum_n b_n|e_n\rangle = \sum_n a_n\hat{Q}|e_n\rangle$$

Taking the inner product with $|e_m\rangle$ with both sides:

$$\sum_n b_n\langle e_m|e_n\rangle = \sum_n a_n\langle e_m|\hat{Q}|e_n\rangle$$

Since we have an orthonormal basis,

$$b_m = \sum_n a_n Q_{mn}$$

Operators have different representations in different bases:

$$\hat{x} \to \begin{cases} x & \text{position space} \\ i\hbar\partial/\partial p & \text{momentum space} \end{cases}$$

$$\hat{p} \to \begin{cases} -i\hbar\partial/\partial x & \text{position space} \\ p & \text{momentum space} \end{cases}$$

Dirac Notation

Ket: are elements of a Hilbert vector space H, denoted by $|a\rangle$; a is merely a label.

A *ket* analogous to a column vector:

$$|\alpha\rangle = \begin{bmatrix} a_1 \\ a_2 \\ \dots \\ a_n \end{bmatrix}$$

Bra: belongs to the dual Hilbert vector space, denoted by $\langle a|$; a is merely a label.

For every ket vector there exists a unique bra, and vice versa. (Riesz representation theorem)

$$|a\rangle \leftrightarrow \langle a|$$
$$\alpha|a\rangle + \beta\langle b| \leftrightarrow \alpha^*\langle a| + \beta^*\langle b|$$

A *bra* is

- returns a complex number, given a vector
- an instruction to integrate (in coordinate notation)

$$\langle f| = \int f^*(\dots)\,dx$$

- analogous to row vectors:

$$\langle\beta| = \begin{bmatrix} b_1^* & b_2^* & \dots & b_n^* \end{bmatrix}$$

Bra-ket: is the Dirac notation for the inner product. Between two kets $|a\rangle$, $|b\rangle$, the braket is $\langle a|b\rangle$

Schwarz inequality: For any two states $|a\rangle$, $|b\rangle$ of the Hilbert space, we can show

$$|\langle a|b\rangle|^2 \leq \langle a|a\rangle \langle b|b\rangle$$

If $|a\rangle = \alpha |b\rangle$ for some scalar, then

$$|\langle a|b\rangle|^2 = \langle a|a\rangle \langle b|b\rangle$$

Triangle inequality: For any two states $|a\rangle$, $|b\rangle$,

$$\sqrt{\langle a+b|a+b\rangle} \leq \sqrt{\langle a|a\rangle} + \sqrt{\langle b|b\rangle}$$

Recall the matrix that projects a vector $\underline{x}$ onto a vector $\underline{u}$ is given by

$$\underline{P} = \frac{\underline{u} \cdot \underline{u}^\intercal}{\|\underline{u}\|^2}$$

where $\underline{u} \cdot \underline{u}^\intercal$ returns a matrix, and is called an *outer product*.

We define the projection operator. For a normalized ket-vector: $|\alpha\rangle$, the operator

$$\hat{P} = |\alpha\rangle\langle\alpha|$$

projects another ket-vector onto the 1-D subspace spanned by $|\alpha\rangle$.

Two states $|a\rangle$, $|b\rangle$ are orthogonal if

$$\langle a|b\rangle = 0$$

Completeness is possible only if the eigenfuntions for a complete basis that spans the space. This basis can always be orthonormalized. So an alternative statement of completeness is that

$$\sum |e_n\rangle\langle e_n| = \mathbb{I}$$

or when the functions are Dirac-orthonormal,

$$\int |e_z\rangle\langle e_z| \, dz = \mathbb{I}$$

- $\mathbb{I} \neq 1$. They are the result of different operations

Forbidden quantities: if $|a\rangle$, $|b\rangle$ belong to the same Hilbert space, then products of the type: $|a\rangle\,|b\rangle$, or $\langle a|\,\langle b|$ are forbidden. They have no meaning *in general*.

Changing bases in Dirac Notation

Let $|x\rangle$, $|p\rangle$, $|n\rangle$ be eigenstates of the position, momentum, and energy (discrete) operator.

The eigenstates are orthonormal, which means that

$$\begin{aligned}\mathbb{I} &= \int dx\, |x\rangle\langle x| \\ &= \int dp\, |p\rangle\langle p| \\ &= \sum |n\rangle\langle n|\end{aligned}$$

If we act on a general quantum state: $|\mathcal{S}(t)\rangle$

$$\begin{aligned}|\mathcal{S}(t)\rangle &= \mathbb{I}\,|\mathcal{S}(t)\rangle \\ &= \int dx\, |x\rangle\,\langle x|\mathcal{S}(t)\rangle & &= \int dx\, |x\rangle\,\Psi(x,t) \\ &= \int dp\, |p\rangle\,\langle p|\mathcal{S}(t)\rangle & &= \int dp\, |p\rangle\,\Phi(p,t) \\ &= \sum_n |n\rangle\,\langle n|\mathcal{S}(t)\rangle & &= \sum |n\rangle\, c_n(t)\end{aligned}$$

We see the componenets of $|\mathcal{S}(t)\rangle$ are expressed as the position-space, momentum-space, and "energy-space" wave functions, in their corresponding basis.

Quantum mechanics in three dimensions

The Schrodinger equation

In three dimensions, the classical Hamiltonian for a single particle is

$$H = \frac{p^2}{2m} + V$$

by substituting

$$p_i \to -i\hbar \frac{\partial}{\partial x_i}$$

we get

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V$$

Schrodinger's equation:

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

- V and Ψ are now functions of $\underline{r} = (x, y, z)$

In three dimensions, the probability of finding the particle in the volume $d^3\underline{r}$ is:

$$|\Psi(\underline{r}, t)|^2 d^3\underline{r}$$

Normalization:

$$\int |\Psi|^2 \, d^3\underline{r} = 1$$

As before, when V is time independent, we can apply separation of variables to find

$$\phi_n(t) = e^{iE_n t/\hbar}$$

and the time-independent equation:

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

whose's solution are eigenstates of the Hamiltonian. The general solution to the time-dependent equation is a superposition of eigenstates:

$$\Psi(\underline{r}, t) = \sum c_n \psi_n(\underline{r}) e^{-iE_n t/\hbar}$$

Spherical coordinates

Using the spherical Laplacian, we can write Schrodinger's equation using spherical coordinates.

Separation of variables looks for

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi)$$

$R(r)$ is the solution to the radial equation:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left(V(r) - E\right) = \ell(\ell+1)$$

and $Y(\theta, \phi)$, *the angular wave function*, is the solution to the angular equation:

$$\frac{1}{Y}\left(\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2 Y}{\partial\phi^2}\right) = -\ell(\ell+1)$$

where $\ell(\ell+1)$ is a the separation constant.

The angular equation

- The angular equation is independent of the central field.

We solve the angular equation by separation of variables:

$$Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$$

Multiply both sides by $Y\sin^2(\theta)$, to find that

$$\sin(\theta)\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)\sin^2(\theta)Y$$

Substituting:

$$\sin(\theta)\frac{\partial}{\partial\theta}\left(\sin(\theta)\Phi\frac{\partial\Theta}{\partial\theta}\right) + \Theta\frac{\partial^2\Phi}{\partial\phi^2} = -\ell(\ell+1)\sin^2(\theta)\Phi\Theta$$

Divide both sides by $\Theta\Phi$:

$$\frac{1}{\Theta}\sin(\theta)\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta}{\partial\theta}\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = -\ell(\ell+1)\sin^2(\theta)$$

Let the separation constant be m^2 (m is any complex number, not mass):

$$\frac{1}{\Theta}\sin(\theta)\frac{d}{d\theta}\left(\sin(\theta)\frac{d\Theta}{d\theta}\right) + \ell(\ell+1)\sin^2(\theta) = m^2$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$$

The ϕ equation has solution:

$$\Phi(\phi) = e^{im\phi}$$

- Let m run from $(-\infty, \infty)$
- Absorb constant into $\Theta(\theta)$
- Require $\Phi(\phi + 2\pi) = \Phi(\phi)$, this implies $m = 0, \pm 1, \pm 2, \ldots$

The θ equation as solution

$$\Theta(\theta) = AP_\ell^m(\cos(\theta))$$

Where $P_\ell^m(x)$ is the *associated Legendre function*

The associated Legendre function:

$$P_\ell^m(x) = (-1)^m \left(1 - x^2\right)^{m/2} \left(\frac{d}{dx}\right)^m P_\ell(x)$$

The Legendre polynomials are given by the *Rodrigues formula*:

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \left(\frac{d}{dx}\right)^\ell \left(x^2 - 1\right)^\ell \qquad \ell \geq 0$$

The first couple of Legendre polynomials are given by

$$P_1(x) = x$$
$$P_2(x) = \left(3x^2 - 1\right)/2$$
$$P_3(x) = \left(5x^3 - 3x\right)/2$$
$$P_4(x) = \left(35x^4 - 30x^2 + 3\right)/8$$
$$P_5(x) = \left(63x^5 - 70x^3 + 15x\right)/8$$

Properties of Legendre polynomials:

- $P_l(1) = 1$
- P_ℓ is a polynomial of degree ℓ

Properties of associated Legendre function:

- $P_\ell^m(x)$ is not a polynomial in general; when m is odd, $(1 - x^2)^{m/2}$ results in a term with a square root
- $P_\ell^m(x)$ is a polynomial in $\cos(\theta)$, or in $\sin(\theta)$ when m is odd
- When $m > \ell$, $P_\ell^m = 0$
- For some ℓ, there exists $2\ell + 1$ values of m such that $P_\ell^m \neq 0$

To normalize $\psi = R(r)Y(\theta, \phi)$:

$$\int |R|^2 |Y|^2 r^2 \sin(\theta)\, dr\, d\theta\, d\phi = 1$$

Implies

$$\int_0^\infty |R|^2 r^2\, dr = 1$$

and

$$\int_0^{2\pi} \int_0^\pi |Y|^2 \sin(\theta)\, d\theta\, d\phi = 1$$

Spherical harmonics: are the normalized angular wave functions:

$$Y_\ell^m(\theta, \phi) = \sqrt{\frac{(2\ell + 1)}{4\pi} \frac{(\ell - 1)!}{(\ell + m)!}} e^{im\phi} P_\ell^m(\cos(\theta))$$

Spherical harmonics are orthogonal:

$$\int_0^\pi \int_0^{2\pi} (Y_\ell^m)^* Y_{\ell'}^{m'} \sin(\theta)\, d\theta\, d\phi = \delta_{\ell\ell'}\delta_{mm'}$$

The radial equation

The central field, $V(r)$ only effects the radial equation.

$$\frac{1}{R}\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left(V(r) - E\right) = \ell(\ell + 1)$$

Multiply both sides by R:

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left(V(r) - E\right) R = \ell(\ell + 1)R$$

Let $u(r) = rR(r)$, we will find that the angular equation reduces to

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{\text{eff}}u = Eu$$

where

$$V_{\text{eff}} = V + \frac{\hbar^2}{2m}\frac{\ell(\ell + 1)}{r^2}$$

is the *effective potential*.

Since the additional term is positive, it can be interpreted as a "repulsive force". This is why its called the *centrifugal term*.

Normalizing R implies normalizing:

$$\int_0^\infty |u|^2\, dr = 1$$

Angular momentum

In classical mechanics, energy and momentum is conserved for motion in a central field.

$$\underline{L} = \underline{r} \times \underline{p}$$

By substituting $\underline{p}$ for the operator $\hat{\underline{p}} = -i\hbar\underline{\nabla}$, and $\underline{r}$ for the position operator, we find the quantum mechanical angular momentum operator

$$\hat{\underline{L}} = i\hbar\hat{\underline{r}} \times \underline{\nabla}$$

with components:

$$\hat{L}_x = y\hat{p}_z - z\hat{p}_y$$
$$\hat{L}_x = z\hat{p}_x - x\hat{p}_z$$
$$\hat{L}_z = x\hat{p}_y - y\hat{p}_x$$

$\hat{\underline{L}}$, and $\hat{\underline{L}}^2$ are both hermitian operators.

Commutation relations

We can verify that

$$\left[x_i, p_j\right] = i\hbar\delta_{ij}$$

and

$$\left[x_i, x_j\right] = \left[p_i, p_j\right] = 0$$

Eigenvalues