PHYS2B22 Quantum Physics
Evening course lecture notes. Set 4.
Sam Morgan 2005

Outline of section 4

The formal basis of quantum mechanics

- Overview of the postulates of quantum mechanics
- Linear Hermitian Operators
  - eigenvalues and eigenvectors
  - orthonormality and completeness
- Predicting results of measurements
  - expectation values
  - collapse of the wavefunction
- Commutation relations
  - compatible observables
  - uncertainty principle
- Wavepackets

Formal basis of quantum mechanics

This section puts quantum mechanics onto a more formal mathematical footing by specifying those *postulates* of the theory which cannot be derived from classical physics.

Main ingredients:

1. The wave function (to represent the state of the system)
2. Hermitian operators and eigenvalues (to represent observables)
3. A recipe for finding the operator associated with an observable
4. A description of the measurement process, and for predicting the distribution of possible outcomes
5. The time-dependent Schrödinger equation for evolving the wavefunction in time

The wave function

Postulate 1: For every dynamical system, there exists a wavefunction Ψ that is a continuous, square-integrable, single-valued function of the coordinates of all the particles and of time, and from which all possible predictions about the physical properties of the system can be obtained.

Examples of the meaning of *"The coordinates of all the particles"*

For a single particle moving in one dimension: $\Psi(x,t)$

For a single particle moving in three dimensions: $\Psi(\mathbf{r},t)$

For two particles moving in three dimensions: $\Psi(\mathbf{r}_1,\mathbf{r}_2,t)$

Square-integrable means that the normalization integral is finite

If we know the wavefunction we know everything it is possible to know.

Observables and operators

Postulate 2a: Every **observable** is represented by a **Linear Hermitian Operator** (LHO).

An operator *L* is *linear* if and only if

$$\hat{L}[c_1 f_1 + c_2 f_2] = c_1\hat{L}[f_1] + c_2\hat{L}[f_2]$$

(for arbitrary functions f_1 and f_2 and constants c_1 and c_2)

Examples: which of the following operators are linear?

$$\hat{L}_1[f] \equiv f + 2$$
$$\hat{L}_2[f] \equiv xf$$
$$\hat{L}_3[f] \equiv \sqrt{x}$$
$$\hat{L}_4[f] \equiv \frac{\mathrm{d}f}{\mathrm{d}x}$$

Note: the operators involved may or may not be *differential operators* (i.e. they may or may not involve differentiating the wavefunction).

Hermitian operators

An operator O is **Hermitian** if and only if

$$\int_{-\infty}^{\infty} f_i^* (\hat{O} f_j)\mathrm{d}x = \left[\int_{-\infty}^{\infty} f_j^* (\hat{O} f_i)\mathrm{d}x\right]^*$$

$$= \int_{-\infty}^{\infty} f_j (\hat{O}^* f_i^*)\mathrm{d}x$$

for **all** functions f_i f_j which vanish at infinity

Special case.
If operator O is real, this is

$$\int_{-\infty}^{\infty} f_i^* (\hat{O} f_j)\mathrm{d}x = \int_{-\infty}^{\infty} f_j (\hat{O} f_i^*)\mathrm{d}x$$

Compare the definition of a Hermitian matrix **M**

$$M_{ij} = \left[M_{ji}\right]^*$$

Analogous if we identify a matrix element with an integral:

$$M_{ij} \Longleftrightarrow \int_{-\infty}^{\infty} f_i^* (\hat{O} f_j)\mathrm{d}x$$

Hermitian operators: examples

$$\int_{-\infty}^{\infty} f_i^* (\hat{O} f_j)\mathrm{d}x = \int_{-\infty}^{\infty} f_j (\hat{O}^* f_i^*)\mathrm{d}x$$

The operator x is Hermitian

The operator $\frac{\mathrm{d}}{\mathrm{d}x}$ is not Hermitian

but $-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}$ is Hermitian

The operator $\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ is Hermitian

Eigenvectors and eigenfunctions

Postulate 2b: the **eigenvalues** of the linear Hermitian operator give the possible results that can be obtained when the corresponding physical quantity is measured.

Definition of an eigenvalue for a general linear operator

$$\boxed{\hat{a}\phi_n = \lambda_n \phi_n}$$

operator

eigenvalue

eigenfunction

Compare definition of an eigenvalue of a matrix $\mathbf{Mx} = \lambda \mathbf{x}$

Example: the time-independent Schrödinger equation:

$$\boxed{\hat{H}\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)}$$

Important fact: The eigenvalues of a Hermitian operator are **real** (like the eigenvalues of a Hermitian matrix). Proof later.

Identifying the operators

Postulate 3: the operators representing the position and momentum of a particle are

$$\hat{x} = x \qquad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

(one dimension)

$$\hat{\mathbf{r}} = \mathbf{r} \qquad \hat{\mathbf{p}} = -i\hbar\left[\mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}\right] = -i\hbar\nabla$$

(three dimensions)

Other operators may be obtained from the corresponding classical quantities by making these replacements everywhere.

Examples:

Kinetic energy $$\mathrm{K}_x = \frac{\mathrm{p}_x^2}{2\mathrm{m}} \Rightarrow \hat{\mathrm{K}}_x = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

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

Angular momentum (see Section 5) $$\mathbf{L} = \mathbf{r}\times\mathbf{p} \rightarrow \hat{\mathbf{L}} = -i\hbar\mathbf{r}\times\nabla$$

Example: Momentum eigenfunctions

Eigenfunction equation

Momentum eigenfunction

$$\hat{p}_x \phi_p(x) = p\phi_p(x)$$

Momentum operator $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$

Eigenvalue = the momentum

$$\boxed{\Rightarrow -i\hbar \frac{\partial}{\partial x}\phi_p(x) = p\phi_p(x)}$$

Eigenfunctions are plane waves $\boxed{\phi_p(x) = e^{ikx} = e^{ipx/\hbar}}$

p = ħk from the de Broglie relation

$$-i\hbar \frac{\partial}{\partial x}\left(e^{ikx}\right) = hk\left(e^{ikx}\right) = p\left(e^{ikx}\right)$$

Important properties of Linear Hermitian Operators

In the eigenvalue equation $\boxed{\hat{Q}\phi_n = q_n\phi_n}$

(i) The eigenvalues are real $\boxed{q_n = q_n^*}$

(ii) Different eigenfunctions are orthogonal

$$\boxed{\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)\,\mathrm{d}x = 0, \quad (m \neq n)}$$

(iii) The eigenfunctions form a complete set $\boxed{\Psi(x,t) = \sum_n a_n(t)\phi_n(x)}$

Important properties of Linear Hermitian Operators (2)

Proof of (i) and (ii)

$$\hat{Q}\phi_n = q_n\phi_n \qquad (1)$$
$$\hat{Q}\phi_m = q_m\phi_m \qquad (2)$$

Reminder: Hermitian property

$$\int_{-\infty}^{\infty} f_i^*(\hat{Q}f_j)\mathrm{d}x = \left[\int_{-\infty}^{\infty} f_j^*(\hat{Q}f_i)\mathrm{d}x\right]^*$$

$$\int \phi_m^* \times (1) \Rightarrow \int \phi_m^* \hat{Q}\phi_n dx = q_n \int \phi_m^* \phi_n dx$$

$$\left[\int \phi_n^* \times (2)\right]^* \Rightarrow \left[\int \phi_n^* \hat{Q}\phi_m dx\right]^* = q_m^* \int \phi_m^* \phi_n dx$$

Use the Hermitian property to show $\left(q_n - q_m^*\right)\int_{-\infty}^{\infty} \phi_m^* \phi_n dx = 0$

Case 1: n = m $\int_{-\infty}^{\infty} \phi_n^* \phi_n dx \neq 0 \Rightarrow q_n = q_n^*$

Can choose normalized eigenfunctions $\int_{-\infty}^{\infty} \phi_n^* \phi_n dx = 1$

Case 2: n ≠ m and $q_n \neq q_m \Rightarrow \int_{-\infty}^{\infty} \phi_m^* \phi_n dx = 0$

Case 3: n ≠ m but $q_n = q_m$ next!

Important properties of Linear Hermitian Operators (3)

Case 3: n ≠ m but $q_n = q_m$ (**degenerate eigenvalues**)

Any linear combination of degenerate eigenfunctions is also an eigenfunction with the same eigenvalue:

$$\begin{aligned}\hat{Q}\left[c_1\phi_1 + c_2\phi_2\right] &= c_1\hat{Q}[\phi_1] + c_2\hat{Q}[\phi_2] \\ &= c_1 q\phi_1 + c_2 q\phi_2 \\ &= q\left[c_1\phi_1 + c_2\phi_2\right]\end{aligned}$$

So we are free to *choose* two linear combinations that are orthogonal, e.g.

$$\phi_a = \phi_1$$
$$\phi_b = c_1\phi_1 + c_2\phi_2$$

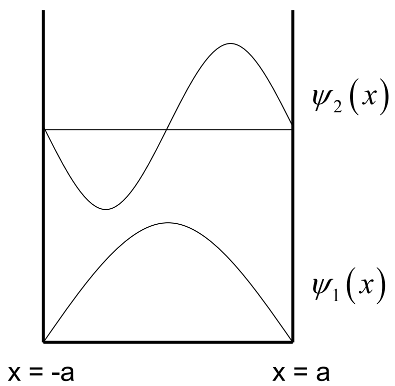
Two coefficients and two constraints: normalization and orthogonality

If the eigenfunctions are all orthogonal *and* normalized, they are said to be **orthonormal**.

$$\int_{-\infty}^{\infty} \phi_m^* \phi_n dx = \delta_{mn} = \begin{cases} 1, & \text{if } m = n \\ 0, & \text{if } m \neq n \end{cases}$$

Orthonormality example: Infinite well

Consider the two lowest energy eigenfunctions of the time-independent Schrödinger equation for an infinite square well



Normalized eigenstates are

$$\psi_1(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{\pi}{2a}x\right)$$
$$\psi_2(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{2\pi}{2a}x\right)$$

$$\frac{1}{a}\int_{-a}^{a}\cos\left(\frac{\pi x}{2a}\right)\sin\left(\frac{2\pi x}{2a}\right)dx = 0$$

We have the integral of an odd function over an even region, which is zero.
The eigenstates are orthogonal because their positive and negative regions give cancelling contributions to the integral.

Orthonormality example: Infinite well (2)

General case

$$\psi_n(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right), \quad n = 1,3,5\ldots\infty$$
$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right), \quad n = 2,4,6\ldots\infty$$

Can easily prove orthonormality using trigonometry formulas

$$\frac{1}{a}\int_{-a}^{a}\sin\left(\frac{n\pi x}{2a}\right)\sin\left(\frac{m\pi x}{2a}\right)dx = \delta_{mn}$$

$$\frac{1}{a}\int_{-a}^{a}\cos\left(\frac{n\pi x}{2a}\right)\cos\left(\frac{m\pi x}{2a}\right)dx = \delta_{mn}$$

$$\frac{1}{a}\int_{-a}^{a}\cos\left(\frac{n\pi x}{2a}\right)\sin\left(\frac{m\pi x}{2a}\right)dx = 0$$

These results are already familiar from Fourier series

Complete sets of functions

The eigenfunctions φ_n of a Hermitian operator form a **complete set**. This means that **any other function satisfying the same boundary conditions can be expanded** as:

$$\boxed{\psi(x) = \sum_n a_n \phi_n(x)}$$

This expansion is a generalization of the Fourier series.
This sum of different eigenstates is called a **superposition**.

If the eigenfunctions are orthonormal, the coefficients a_n can be found as follows (in 1D)

$$\boxed{a_n = \int_{-\infty}^{\infty} \phi_n^*(x)\psi(x)\,dx}$$

Proof

$$\int_{-\infty}^{\infty} \phi_n^*(x)\psi(x)\,dx = \int_{-\infty}^{\infty} \phi_n^*(x)\sum_m a_m \phi_m(x)\,dx$$

$$= \sum_m a_m \int_{-\infty}^{\infty} \phi_n^*(x)\phi_m(x)\,dx = a_n$$

Orthonormality

$$\boxed{\int_{-\infty}^{\infty} \phi_n^* \phi_m\,dx = \delta_{mn}}$$

These expansions are very important in describing the measurement process.

Completeness for a continuum

Particles can have a discrete set of eigenvalues (like the harmonic oscillator or infinite potential well) or they can have a continuum of energies (e.g. a free particle).

For a continuum, use an integral instead of a sum in the wavefunction expansion

$$\boxed{\psi(x) = \sum_n a_n \phi_n(x) \rightarrow \psi(x) = \int_{-\infty}^{\infty} a(k)\phi(k,x)\,dk}$$

$$\boxed{a(k) = \int_{-\infty}^{\infty} \phi^*(k,x)\psi(x)\,dx}$$

E.g. Free particles: Use momentum eigenstates

$$\psi(x) = \int_{-\infty}^{\infty} a(k)\frac{e^{ikx}}{\sqrt{2\pi}}\,dk, \quad a(k) = \int_{-\infty}^{\infty} \frac{e^{-ikx}}{\sqrt{2\pi}}\psi(x)\,dx$$

This is just a Fourier decomposition

Expansion in complete sets: examples

A particle is in an infinite well from –a to a. For the wavefunctions given, find the coefficients a_n in an expansion using the Hamiltonian eigenstates (the wavefunctions are zero outside the well of course).

1) $$\psi(x) = \frac{1}{3\sqrt{a}}\left[\cos\left(\frac{\pi x}{2a}\right) + \sqrt{3}\sin\left(\frac{2\pi x}{2a}\right) + \sqrt{5}\cos\left(\frac{5\pi x}{2a}\right)\right]$$

2) $$\psi(x) = \frac{1}{\sqrt{2a}}$$

Hamiltonian eigenstates

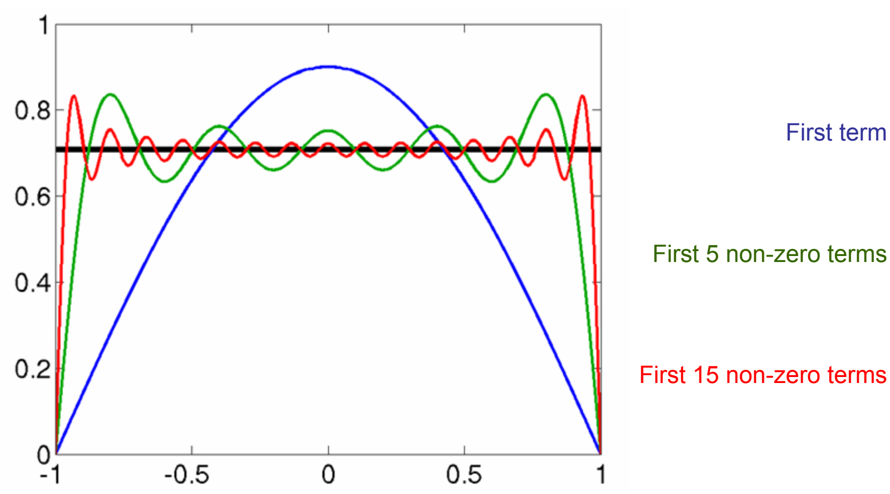
$$\psi_n(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right), \quad n = 1,3,5\ldots\infty$$
$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right), \quad n = 2,4,6\ldots\infty$$

$$\psi(x) = \sum_n a_n\phi_n(x)$$

$$a_n = \int_{-a}^{a}\phi_n^*(x)\psi(x)\,dx$$

Expansion in complete sets: examples

Plot of partial expansions of $\psi(x) = \frac{1}{\sqrt{2a}}$



Eigenfunctions and measurement

Postulate 4a: When a measurement of the observable Q is made on a normalized wavefunction ψ, the probability of obtaining the eigenvalue q_n is given by the **modulus squared of the overlap integral**

$$\Pr(q_n) = |a_n|^2, \quad a_n = \int_{-\infty}^{\infty} \phi_n^*(x)\psi(x)\,dx$$

This corresponds to expanding the wavefunction in the complete set of eigenstates of the operator for the physical quantity we are measuring and interpreting the modulus squared of the expansion coefficients as the probability of getting a particular result. This is the general form of the Born interpretation

$$\psi(x) = \sum_n a_n\phi_n(x).$$

Corollary: if a system is *definitely* in the eigenstate φ_n, the result of measuring Q is *definitely* the corresponding eigenvalue q_n.

The meaning of these "probabilities" for a single system is still a matter for debate. The usual interpretation is that the probability of a particular result determines the frequency of that result in measurements on an ensemble of similar systems.

Expectation values

The expectation value is the average (mean) value of many measurements. It is the sum of all the possible results times the corresponding probabilities:

$$\langle Q\rangle = \sum_n \Pr(q_n)q_n = \sum_n |a_n|^2 q_n$$

We can also write this as:

$$\langle Q\rangle = \int_{-\infty}^{\infty} \psi^*(x)\hat{Q}\psi(x)\,dx$$

Proof

Expand Ψ in eigenstates of Q

$$\psi(x) = \sum_n a_n\phi_n(x)$$

$$\hat{Q}\phi_n = q_n\phi_n$$

$$\int dx\,\phi_n^*\phi_m = \delta_{mn}$$

$$\langle Q\rangle = \int\left[\sum_m a_m^*\phi_m^*\right]\hat{Q}\left[\sum_n a_n\phi_n\right]dx$$

$$= \int\left[\sum_m a_m^*\phi_m^*\right]\left[\sum_n a_n q_n\phi_n\right]dx$$

$$= \sum_m\sum_n a_m^* a_n q_n \int \phi_m^*\phi_n\,dx = \sum_n |a_n|^2 q_n$$

Wavefunction Normalization

The normalization of the wavefunction is $N = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\,dx = 1$

We can also write this in terms of the expansion coefficients $\sum_n |a_n|^2 = 1$ for a normalized wavefunction

This is consistent with the probability interpretation for expansion coefficients $\Pr(q_n) = |a_n|^2 \Rightarrow \sum_n |a_n|^2 = 1$

Can prove this using the expectation value of the operator Q = 1!
The eigenvalues of Q = 1 are q_n = 1 so we have

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^*(x)\hat{Q}\psi(x)\,dx, \quad \langle Q \rangle = \sum_n |a_n|^2 q_n$$

$$\langle 1 \rangle = \int_{-\infty}^{\infty} \psi^*(x) 1 \psi(x)\,dx = 1, \quad \langle 1 \rangle = \sum_n |a_n|^2 = 1$$

Expectation Values: examples

$$\psi_n(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right), \quad n = 1,3,5\ldots\infty$$

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right), \quad n = 2,4,6\ldots\infty$$

$$E_n = \frac{n^2\hbar^2\pi^2}{8ma^2}$$

1) A particle is in the ground state of an infinite well from –a to a.
What is the expectation value of the position and the momentum?

2) For the same infinite well, a particle has wavefunction

$$\psi(x) = \frac{1}{3\sqrt{a}}\left[\cos\left(\frac{\pi x}{2a}\right) + \sqrt{3}\sin\left(\frac{2\pi x}{2a}\right) + \sqrt{5}\cos\left(\frac{5\pi x}{2a}\right)\right]$$

Check that this is correctly normalized.
What is the expectation value of the energy?

Expectation Values: examples

3) A particle is in the ground state of a harmonic oscillator potential of frequency ω:

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

Calculate the average value of its kinetic energy. You may use:

$$\int_{-\infty}^{\infty} \exp\left(-x^2/a^2\right)dx = a\sqrt{\pi} \qquad \int_{-\infty}^{\infty} x^2 \exp\left(-x^2/a^2\right)dx = \frac{a^3\sqrt{\pi}}{2}$$

Collapse of the wavefunction

Postulate 4b: Immediately after a measurement, the wavefunction is an eigenfunction of the operator corresponding to the eigenvalue just obtained as the measurement result.

$$\boxed{\psi(x) = \sum_n a_n \phi_n(x) \rightarrow \psi(x) = \phi_n(x)} \qquad \boxed{\Pr = |a_n|^2}$$

This is the famous **collapse of the wavefunction** and is an idea mainly due to John von Neumann in 1932.

This ensures that we are guaranteed to get the same result if we immediately re-measure the same quantity.

$$\boxed{\psi(x) = \phi_n(x) \Rightarrow \Pr(q_n) = |a_n|^2 = 1}$$

Problem: This is a different time-evolution from the Schrödinger equation. How do we know when to use the Schrödinger equation and when to use collapse, i.e. what constitutes a measurement?

A 'folk tale' for quantum measurement ….

A quantum state in a superposition is like a mythical beast, a Chimera, which is part lion, part goat…

Problem: is it a goat or a lion?

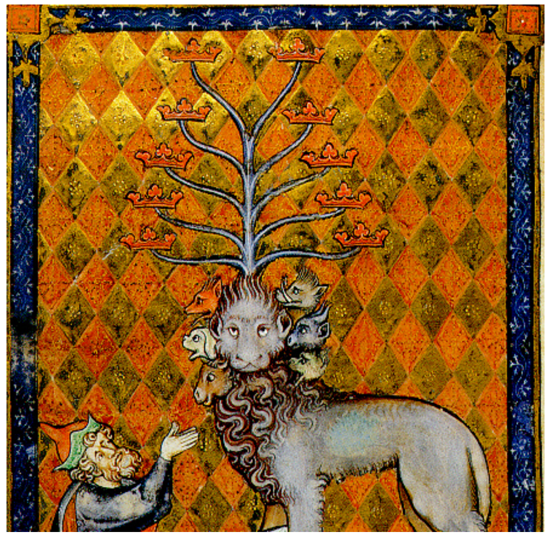
Make a measurement!

Offer the Chimera a cabbage and a steak.

If it takes the cabbage, it is definitely a goat. If it takes the steak, it is definitely a lion…

Actually, of course, it is neither. It is a superposition!

It behaves like a goat if you treat it like a goat and like a lion if you treat it like a lion (rather like particle-wave duality, cf. the double-slit experiment!)



Evolution of the system

Postulate 5: Between measurements (i.e. when it is not disturbed by external influences) the wavefunction evolves with time according to the time-dependent Schrödinger equation.

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

Hamiltonian operator.

This is a linear, homogeneous differential equation, so the linear combination of any two solutions is also a solution.

This is the **superposition principle**.

$$i\hbar\frac{\partial\Psi_1}{\partial t} = \hat{H}\Psi_1$$

$$i\hbar\frac{\partial\Psi_2}{\partial t} = \hat{H}\Psi_2$$

$$\Rightarrow \quad i\hbar\frac{\partial\left(\Psi_1+\Psi_2\right)}{\partial t} = \hat{H}\left(\Psi_1+\Psi_2\right)$$

Time dependent expansions

We can expand the full time-dependent wavefunction using time-dependent expansion coefficients.

$$\boxed{\Psi(x,t) = \sum_n a_n(t)\phi_n(x)}$$

We can work out how these evolve using the TDSE for Ψ(x,t) and the overlap integral.

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

Simple special case:

Suppose the Hamiltonian is time-independent. We know that separated solutions of the TDSE exist in the form:

$$\boxed{\Psi(x,t) = \exp(-iE_n t/\hbar)\psi_n(x)}$$

$$\boxed{\hat{H}\psi_n(x) = E_n\psi_n(x)}$$

The eigenfunctions of the TISE form a complete set, so we can expand the initial wavefunction as

$$\boxed{\Psi(x,0) = \sum_n a_n(0)\psi_n(x)}$$

Hence we can find the complete time dependence from the superposition principle

$$\boxed{\Psi(x,t) = \sum_n \underbrace{a_n(0)\exp(-iE_n t/\hbar)}_{a_n(t)}\psi_n(x)}$$

Commutators

In general operators do not *commute:* the order in which the operators act on functions matters.

$$\boxed{\hat{Q}\hat{R}\psi \neq \hat{R}\hat{Q}\psi \text{ (in general)}}$$

Example, position and momentum operators:

$$\hat{x} = x \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

$$\hat{x}\hat{p}_x\psi = x\left(-i\hbar\frac{\partial}{\partial x}\right)\psi = -i\hbar x\frac{\partial\psi}{\partial x}$$

$$\hat{p}_x\hat{x}\psi = \left(-i\hbar\frac{\partial}{\partial x}\right)(x\psi) = -i\hbar\psi - i\hbar x\frac{\partial\psi}{\partial x}$$

We define the **commutator** as the difference between the two orderings: →

$$\boxed{\left[\hat{Q},\hat{R}\right] \equiv \hat{Q}\hat{R} - \hat{R}\hat{Q}}$$

Two operators commute only if their commutator is zero.

For position and momentum: $[\hat{x},\hat{p}_x]\psi = i\hbar\psi$ ⇒ $\boxed{[\hat{x},\hat{p}_x] = i\hbar}$

Compatible operators

$$\hat{Q}\phi_n = q_n\phi_n$$
$$\hat{R}\phi_n = r_n\phi_n$$

Two observables are **compatible** if their operators share the same eigenfunctions (but not necessarily the same eigenvalues).

Consequence: two compatible observables can have precisely-defined values simultaneously.

Start with general wavefunction $\psi(x) = \sum_n a_n\phi_n(x).$

Measure observable Q. Get result q_m with (probability $|a_m|^2$) → Wavefunction collapses to corresponding eigenfunction φ_m → Measure observable R. **Definitely** get r_m (eigenvalue of R for φ_m)

$$\psi(x) = \sum_n a_n\phi_n(x) \to \phi_m(x)$$

→ Wavefunction is still φ_m → Re-measure Q. **Definitely** get q_m again

$$\psi(x) = \phi_m(x)$$

For simplicity we only consider the non-degenerate case here.

Compatible operators (2)

Compatible operators commute

$$\psi(x) = \sum_n a_n\phi_n(x)$$

$$\hat{Q}\phi_n = q_n\phi_n$$
$$\hat{R}\phi_n = r_n\phi_n$$

Proof Expand ψ in the set of simultaneous eigenfunctions

$$\begin{aligned}\left(\hat{Q}\hat{R} - \hat{R}\hat{Q}\right)\psi &= \sum_n a_n\left(\hat{Q}\hat{R} - \hat{R}\hat{Q}\right)\phi_n \\ &= \sum_n a_n\left(\hat{Q}r_n\phi_n - \hat{R}q_n\phi_n\right) \\ &= \sum_n a_n\left(r_nq_n\phi_n - q_nr_n\phi_n\right) = 0\end{aligned}$$

$$\boxed{\begin{aligned}&\Rightarrow \left(\hat{Q}\hat{R} - \hat{R}\hat{Q}\right)\psi = 0 \\ &\Rightarrow \left[\hat{Q}, \hat{R}\right] = 0\end{aligned}}$$

Can also prove the converse (see Rae Chapter 4) :
if two operators commute then they are compatible.

Example: position and momentum

x and p_x do not commute.
There are no functions which are simultaneous eigenfunctions of the position and momentum operators

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

This is directly related to the uncertainty principle.
If we measure x we lose information about p_x and vice versa

$$\boxed{\Delta x\Delta p_x \geq \frac{\hbar}{2}}$$

But now consider $\left[\hat{x},\hat{p}_y\right]\psi = x\left(-i\hbar\frac{\partial\psi}{\partial y}\right)-\left(-i\hbar\frac{\partial}{\partial y}\left[x\psi\right]\right)$

$$= -i\hbar x\frac{\partial\psi}{\partial y}+i\hbar x\frac{\partial\psi}{\partial y}=0$$

$$\boxed{\left[\hat{x},\hat{p}_y\right]=0}$$

So x and p_y commute. The x position and y momentum are compatible.
We can know x and p_y at the same time with arbitrary accuracy.

Commutation relations and the Uncertainty Principle

How does $\left[\hat{x},\hat{p}_x\right]=i\hbar$ relate to the Uncertainty Principle?

$$\boxed{\Delta x\Delta p_x \geq \frac{\hbar}{2}}$$

<u>Outline derivation of the UP</u> (see Rae §4.5)

Define rms deviations

$$(\Delta x)^2 = \left\langle (x-\bar{x})^2\right\rangle$$
$$(\Delta p_x)^2 = \left\langle (p_x-\bar{p}_x)^2\right\rangle$$

Use Schwarz's Inequality to obtain

$$\Delta x\Delta p_x \geq \frac{1}{2}\left|\left\langle\left[\hat{x},\hat{p}_x\right]\right\rangle\right| = \frac{1}{2}\left|\left\langle i\hbar\right\rangle\right|$$
$$\Rightarrow \Delta x\Delta p_x \geq \frac{\hbar}{2}$$

In general we get an uncertainty relation for any two incompatible observables, i.e. whose corresponding operators do not commute

For general non-commuting operators $\hat{Q},\hat{R}$

$$\Delta q\Delta r \geq \tfrac{1}{2}\left|\left\langle\left[\hat{Q},\hat{R}\right]\right\rangle\right|$$

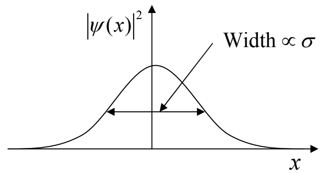
Wavepackets and the Uncertainty Principle

Wavepackets are the best way of describing a quantum system with both particle-like and wave-like characteristics.

We cannot have absolute certainty of both position and momentum. But we can construct a wavepacket which is localized in both position and momentum

E.g. real space probability density

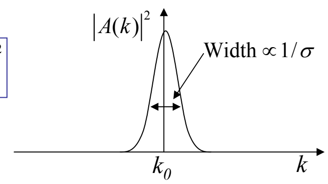
$$\psi(x) \propto e^{ik_0 x} \exp\left(-x^2/4\sigma^2\right)$$
$$|\psi(x)|^2 \propto \exp\left(-x^2/2\sigma^2\right)$$



Write this as a Fourier transform (expansion in momentum eigenstates)

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$
$$\Rightarrow A(k) \propto e^{-\sigma^2 (k-k_0)^2}$$

$$|A(k)|^2 \propto e^{-2\sigma^2 (k-k_0)^2}$$



Wavepackets and the Uncertainty Principle (2)

$$|\psi(x)|^2 \propto e^{-x^2/2\sigma^2}$$
$$|A(k)|^2 \propto e^{-2\sigma^2 (k-k_0)^2}$$

Rough uncertainty in *postion* given from the point where the Gaussian falls to 1/e of its peak value

$$\Delta x = \sqrt{2\sigma^2}$$

Similarly, rough uncertainty in momentum:

$$\Delta k = \sqrt{\frac{1}{2\sigma^2}} \Rightarrow \Delta p = \hbar \Delta k = \hbar \sqrt{\frac{1}{2\sigma^2}}$$

Hence the product of uncertainties is a constant, independent of σ

$$\Delta p \Delta x = \hbar \sqrt{\frac{1}{2\sigma^2}} \sqrt{2\sigma^2} = \hbar$$

NB: The Uncertainty relation is usually evaluated using rms widths rather than our 1/e estimate. In that case we get

$$\Delta p \Delta x = \frac{\hbar}{2}$$

So the Gaussian is actually a minimum uncertainty wavepacket

Summary of the Uncertainty Principle

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

We have now seen *three* ways of thinking about the Uncertainty principle:

(1) As the necessary disturbance of the system due to measurements (e.g. the Heisenberg microscope)

(2) Arising from the properties of Fourier transforms (narrow spatial wavepackets need a wide range of wavevectors in their Fourier transforms and vice versa)

(3) As a fundamental consequence of the fact that *x* and *p* are not compatible quantities so their corresponding Hermitian operators do not commute. They do not share any eigenvectors and therefore cannot have precisely defined values simultaneously.

For general non-commuting operators $\hat{Q}, \hat{R}$

$$\Delta q \Delta r \geq \tfrac{1}{2}\left|\left\langle\left[\hat{Q},\hat{R}\right]\right\rangle\right|$$

Evolution of expectation values

Consider the rate of change of the expectation value of an observable Q for a time-dependent wavefunction

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

$$i\hbar\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} = i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\Psi^*(\hat{Q}\Psi)\mathrm{d}x$$

$$= \int_{-\infty}^{\infty} i\hbar\frac{\partial\Psi^*}{\partial t}(\hat{Q}\Psi) + \Psi^*(i\hbar\frac{\partial\hat{Q}}{\partial t}\Psi) + \Psi^*(\hat{Q}i\hbar\frac{\partial\Psi}{\partial t})\mathrm{d}x$$

$$= \int_{-\infty}^{\infty} -(\hat{H}\Psi^*)(\hat{Q}\Psi) + \Psi^*(\hat{Q}\hat{H}\Psi)\mathrm{d}x + i\hbar\left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

$$= \int_{-\infty}^{\infty} -\Psi^*\hat{H}(\hat{Q}\Psi) + \Psi^*(\hat{Q}\hat{H})\Psi\mathrm{d}x + i\hbar\left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

$$= -\left\langle\left[\hat{H},\hat{Q}\right]\right\rangle + i\hbar\left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \qquad -i\hbar\frac{\partial\Psi^*}{\partial t} = \hat{H}\Psi^*$$

$$\int_{-\infty}^{\infty} f_i^*(\hat{H}f_j)\mathrm{d}x = \int_{-\infty}^{\infty} f_j(\hat{H}f_i^*)\mathrm{d}x$$

$$\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

Ehrenfest's theorem

Example: conservation of energy

Consider the rate of change of the mean energy

$$\boxed{\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle}$$

$$\frac{d\langle E\rangle}{dt} = \frac{\partial}{\partial t}\int_{-\infty}^{\infty}\Psi^*\hat{H}\Psi\mathrm{d}x$$

$$= \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{H}\right]\right\rangle + \left\langle\frac{\partial\hat{H}}{\partial t}\right\rangle$$

The Hamiltonian is independent of time $\left\langle\frac{\partial\hat{H}}{\partial t}\right\rangle = 0$

Everything commutes with itself! $\left[\hat{H},\hat{H}\right] = 0$

$$\Rightarrow \quad \boxed{\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}t} = 0}$$

Although the energy of a system may be uncertain (in the sense that measurements made on many copies of the system may give different results) the average energy is always conserved with time.

Example: position and momentum

Consider the rate of change of the mean position

$$\boxed{\frac{d\langle x\rangle}{dt} = \frac{\partial}{\partial t}\int_{-\infty}^{\infty}\Psi^* x\Psi\mathrm{d}x = \frac{i}{\hbar}\left\langle\left[\hat{H},x\right]\right\rangle + \left\langle\frac{\partial x}{\partial t}\right\rangle}$$

$$\boxed{\left\langle\frac{\partial x}{\partial t}\right\rangle = 0}$$

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\left\langle\left[\frac{\hat{p}^2}{2m} + V(x), x\right]\right\rangle$$

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

$$\boxed{\left[V(x),x\right] = 0}$$

$$= \frac{i}{\hbar}\left\langle\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}, x\right]\right\rangle$$

$$\boxed{\left[\frac{d^2}{dx^2}, x\right] = 2\frac{d}{dx}}$$

$$= \left\langle\frac{-i\hbar}{m}\frac{d}{dx}\right\rangle = \left\langle\frac{\hat{p}_x}{m}\right\rangle$$

Can also show similarly that $\boxed{\frac{\mathrm{d}\langle p_x\rangle}{\mathrm{d}t} = -\left\langle\frac{dV(x)}{dx}\right\rangle}$

These look very like the usual classical expressions relating position and velocity and Newton's second law. So we recover classical mechanics-like expressions for the evolution of expectation values.

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Sam Morgan 2005

Summary (1)

There is a wavefunction

Linear Hermitian Operators represent observables
Eigenvalues give possible measurement results

$$\int_{-\infty}^{\infty} f_i^*(\hat{O} f_j)\mathrm{d}x = \int_{-\infty}^{\infty} f_j(\hat{O}^* f_i^*)\mathrm{d}x$$

$$\hat{Q}\phi_n = q_n\phi_n$$

Orthonormality of eigenfunctions $\int_{-\infty}^{\infty} \phi_m^* \phi_n dx = \delta_{mn}$

Completeness and the overlap integral

$$\Psi(x,t) = \sum_n a_n(t)\phi_n(x)$$

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

Position and momentum operators
Other operators: use these in the classical expression

$$\hat{x} = x \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

Collapse of the wavefunction at a measurement

$$\psi(x) = \sum_n a_n\phi_n(x) \rightarrow \psi(x) = \phi_n(x)$$

$$\Pr = |a_n|^2$$

Summary (2)

Expectation values

and Ehrenfest's theorem

$$\langle Q\rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q}\Psi dx = \sum_n |a_n|^2 q_n$$

$$\frac{\mathrm{d}\langle Q\rangle}{\mathrm{d}t} = \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

Normalization $\sum_n |a_n|^2 = 1$

Time-dependent Schrödinger equation $i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$

Commutation relations

and the Uncertainty principle

$$\left[\hat{Q},\hat{R}\right] \equiv \hat{Q}\hat{R} - \hat{R}\hat{Q} \qquad \left[\hat{x},\hat{p}_x\right] = i\hbar$$

$$\Delta q\Delta r \geq \tfrac{1}{2}\left|\left\langle\left[\hat{Q},\hat{R}\right]\right\rangle\right|$$

Compatible observables:

- Commute
- Have simultaneous eigenfunctions
- Can be uniquely determined simultaneously