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Glossary for Book 1

Number or numbers in parentheses are page references to Book 1.

Italicized words are cross-references to other entries in this Glossary.

addition rule for probability (228) This rule states that the *probability* of obtaining one or other of a set of *mutually exclusive outcomes* in a single trial or experiment is the sum of their individual probabilities.

alpha decay (203) A form of radioactive decay in which the *nucleus* of an atom ejects an energetic *alpha particle*. As a result, the *atomic number* Z of the emitting nucleus is reduced by two, and its *mass number* A is reduced by four. Alpha decay involves the *tunnelling* of alpha particles through a *Coulomb barrier*. See also *Geiger–Nuttall relation*.

alpha particle (12) A type of composite particle, consisting of two *protons* and two *neutrons*, that is emitted in the radioactive decay process known as *alpha decay*. An alpha particle is identical to a helium-4 *nucleus* ($^4_2$He).

amplitude (17, 125) For a sinusoidal *plane wave* described by the function $u(x,t) = A\cos(kx + \omega t + \phi)$, or for a *simple harmonic oscillation* $u(t) = A\cos(\omega t + \phi)$, the positive constant A is called the amplitude of the wave or oscillation. This is the maximum deviation of u from zero.

angular frequency (17, 126) The rate of change of the *phase* of an oscillation or wave. The angular frequency ω is given by

$$\omega = 2\pi f = \frac{2\pi}{T},$$

where f is the *frequency* and T is the *period* of the oscillation or wave. The SI unit of angular frequency is the inverse second, s^{-1}.

arbitrary constant (218) A constant that appears in the *general solution of a differential equation* but does not appear in the *differential equation* itself. The general solution of a differential equation of *order* n contains n arbitrary constants. The arbitrary constants serve to distinguish one *particular solution* from another.

Argand diagram (212) Another term for the *complex plane*.

argument of a complex number (213) Another term for the *phase* of a *complex number*.

atomic number (12) The number, Z, of *protons* in the *nucleus* of an atom, and hence the number of *electrons* in the neutral atom. A chemical element is identified by its atomic number, Z, which determines its chemical properties. Hydrogen, helium and lithium have $Z = 1$, 2 and 3, respectively.

attenuation coefficient (199) A quantity that determines the rate of exponential decrease of some other quantity with increasing distance. An example is the quantity α that appears in the contribution $C\mathrm{e}^{-\alpha x}$ to an *energy eigenfunction* $\psi(x)$ where x is the distance penetrated into a *classically forbidden region*. The SI unit of an attenuation coefficient is m^{-1}.

auxiliary equation (219) An algebraic equation obtained when a trial solution containing undetermined parameters is substituted into a *differential equation*. The auxiliary equation determines possible values of these parameters.

average value (228) If a quantity A is measured N times in a given situation, and the result A_i is obtained on N_i occasions, the average value of A over the set of measurements is defined to be

$$\overline{A} = \frac{1}{N}\sum_{i=1}^{N} N_i A_i = \sum_{i=1}^{N} f_i A_i,$$

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where the sum is over all the possible outcomes and $f_i = N_i/N$ is the *relative frequency* of outcome i.

The measured average value is expected to approach the theoretical *expectation value* as the number of measurements becomes very large. Also called the *mean value*.

barn (196) A unit of area widely used in the measurement of *total cross-sections* in particle and nuclear physics. $1\,\text{barn} = 10^{-28}\,\text{m}^2$.

barrier penetration (88, 133) The quantum phenomenon in which particles may be detected in a *classically forbidden region.*

beam intensity (183) See *intensity*.

beam splitter (15) A device that splits a beam of particles into two or more distinct sub-beams. A *half-silvered mirror* achieves this for a beam of *photons*.

Born's rule (24) For a single particle in one dimension, in a *state* described by the *wave function* $\Psi(x,t)$, Born's rule states that the *probability* of finding the particle at time t in a small interval δx, centred on position x, is

$$\text{probability} = |\Psi(x,t)|^2\,\delta x.$$

For a single particle in three dimensions, in a state described by the wave function $\Psi(\mathbf{r},t)$, the probability of finding the particle at time t in a small volume element δV, centred on position $\mathbf{r}$, is

$$\text{probability} = |\Psi(\mathbf{r},t)|^2\,\delta V.$$

Born's rule is also called 'Born's interpretation of the wave function'.

Born's rule for momentum (170) For a one-dimensional *free-particle wave packet*,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} A(k)\,\mathrm{e}^{\mathrm{i}(kx - E_k t/\hbar)}\,\mathrm{d}k,$$

Born's rule for momentum states that the *probability* of finding the momentum to lie in a small interval $\hbar\,\delta k$, centred on $\hbar k$, is $|A(k)|^2\,\delta k$, where $A(k)$ is the *momentum amplitude*.

The momentum amplitude is independent of time for a free particle, but this is not true for a particle subject to forces. More generally, Born's rule for momentum states that the probability of finding the momentum at time t to lie in a small interval $\hbar\,\delta k$, centred on $\hbar k$, is $|A(k,t)|^2\,\delta k$, where $A(k,t)$ is the momentum amplitude at time t, given by the *Fourier transform* of the *wave function*.

boundary conditions (221) Any conditions that give extra information about the solutions of a *differential equation*. Such information may be sufficient to determine all the *arbitrary constants* in the *general solution of a differential equation*, and so select a unique *particular solution*, or it may determine the *eigenvalues* and *eigenfunctions* of an *eigenvalue equation*.

bound state (91) A *stationary state* in which one part of a *system* is always found in close proximity to another part of the same system. Bound states have discrete *energy eigenvalues*, which lie below the energies of *states* of the system in which the two parts are infinitely far apart.

Cartesian form of a complex number (213) A *complex number* z is said to be expressed in Cartesian form if it is written as $z = x + \mathrm{i}y$, where x and y are *real numbers*.

classical limit (160) Conditions under which the predictions of *quantum mechanics* approach those of *classical mechanics*. The classical limit generally involves objects that are much larger than atoms, and forces that vary smoothly over the width of the *wave packet* describing the object. See also *correspondence principle* and *Ehrenfest's theorem*.

classical mechanics (7) A theory of the behaviour of systems of particles based on Newton's laws. Also called Newtonian mechanics. Fundamental equations in classical mechanics can be expressed in terms of the *Hamiltonian function*.

classical physics (7) A term given to branches of physics that do not rely on quantum ideas. Classical physics embraces *classical mechanics* and subjects such as classical electromagnetism, fluid mechanics and thermodynamics. Most physicists regard special and general relativity as belonging to classical physics, which implies that the major revolution of twentieth-century physics was *quantum physics*, not relativity.

classically forbidden region (66) A region of space from which a particle is excluded by *classical mechanics*. The exclusion arises because the fixed total energy of the particle is less than the value of the *potential energy function* throughout the classically forbidden region.

coefficient rule (105) This rule states that, if the *wave function* $\Psi(x,t)$ of a *system* is expressed as a discrete *linear combination* of *normalized energy eigenfunctions*:

$$\Psi(x,t) = c_1(t)\,\psi_1(x) + c_2(t)\,\psi_2(x) + \dots\,,$$

then the *probability* of obtaining the ith *eigenvalue* E_i is

$$p_i = |c_i(t)|^2\,,$$

where $c_i(t)$ is the coefficient of the ith energy eigenfunction in the wave function at the instant of measurement.

This rule can be extended to any *observable* A, with a discrete set of possible values provided that the wave function is expanded as a linear combination of eigenfunctions of the corresponding quantum-mechanical *operator* $\widehat{\mathrm{A}}$.

collapse of the wave function (27, 97) The abrupt and unpredictable change in a *wave function* that arises during an act of measurement. This collapse cannot be described by *Schrödinger's equation*. An example is the collapse that occurs when the position of a particle is measured by a *Geiger counter*; immediately after the Geiger counter has clicked, the wave function describing the particle is localized in the vicinity of the Geiger counter.

commuting operators (138) Two *operators* $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{B}}$ are said to commute with one another if the effect of applying $\widehat{\mathrm{B}}$ followed by $\widehat{\mathrm{A}}$ is always the same as the effect of applying $\widehat{\mathrm{A}}$ followed by $\widehat{\mathrm{B}}$. In this case, the *commutator* of $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{B}}$ is equal to zero.

commutation relation (138) An equation that specifies the *commutator* of two given *operators*.

commutator (138) The commutator of two *operators* $\widehat{\mathrm{A}}$ and $\widehat{\mathrm{B}}$ is the operator defined by $\widehat{\mathrm{A}}\widehat{\mathrm{B}} - \widehat{\mathrm{B}}\widehat{\mathrm{A}}$.

complete set of functions (164) A discrete set of functions, $\phi_i(x)$ labelled by the index i, is said to be complete if it is possible to expand any reasonable function $f(x)$ in the form

$$f(x) = \sum_i a_i\, \phi_i(x),$$

where the coefficients a_i are constants (independent of x). The *harmonic-oscillator* energy *eigenfunctions* are complete in this sense.

This definition can be extended to a continuous set of functions $\phi_k(x)$, labelled by a continuous index k, by replacing the sum by an integral

$$f(x) = \int_{-\infty}^{\infty} A(k)\, \phi_k(x)\, \mathrm{d}k,$$

where $A(k)$ is some complex-valued function. The *momentum eigenfunctions* are complete in this sense.

complete set of outcomes (228) A set of *mutually exclusive outcomes* for an experiment or trial is said to be complete if every possible outcome of the experiment or trial is a member of the set.

complex conjugate (212) For a given *complex number* z, the complex conjugate z^* is the complex number obtained by reversing the sign of i wherever it appears in z. So, given a complex number

$$z = x + \mathrm{i}y = r(\cos\theta + \mathrm{i}\sin\theta) = r\mathrm{e}^{\mathrm{i}\theta},$$

the complex conjugate is

$$z^* = x - \mathrm{i}y = r(\cos\theta - \mathrm{i}\sin\theta) = r\mathrm{e}^{-\mathrm{i}\theta}.$$

complex number (210) An entity that can be written in the form

$$z = x + \mathrm{i}y,$$

where x and y are *real numbers* and $\mathrm{i} = \sqrt{-1}$. Complex numbers obey the ordinary rules of algebra, with the extra rule that $\mathrm{i}^2 = -1$.

complex plane (212) A plane in which *complex numbers* in the *Cartesian form* $z = x + \mathrm{i}y$ are represented by points with Cartesian coordinates (x, y). *Real numbers* are represented by points along the (horizontal) x-axis, and *imaginary numbers* are represented by points along the (vertical) y-axis. Also called the *Argand diagram*.

conservation of energy (105) In *classical physics*, the principle that the energy of any isolated *system* remains constant in time.

In *quantum physics*, where a system may have an indefinite energy, the principle that the *probability distribution* of energy, in any isolated system, remains constant in time.

constructive interference (30) The phenomenon in which two or more waves reinforce one another when they are superimposed at a given point.

continuity boundary conditions (68) *Boundary conditions* that refer to the continuity of *energy eigenfunctions* and their derivatives. The eigenfunction $\psi(x)$ is always continuous. The first derivative $\mathrm{d}\psi/\mathrm{d}x$ is continuous in regions where the *potential energy function* is finite; it need not be continuous at points where the potential energy function becomes infinite.

continuum (12) The name given to an infinite set of *energy levels* over which the energy varies continuously. The *state* of a particle in the continuum cannot be described by a single *stationary-state wave function* because such a function cannot be *normalized*; instead, it is described by a *wave packet* of indefinite energy.

correspondence principle (135) The general principle that the predictions of *quantum mechanics* should approach those of *classical mechanics* in the limit of high *quantum numbers*. See also *classical limit*.

Coulomb barrier (204) The repulsive barrier, described by the *potential energy function*

$$V(r) = \frac{Qq}{4\pi\varepsilon_0 r},$$

that is encountered by a particle of charge q when it is a distance r from a fixed point-like charge Q, where q and Q have the same sign. The constant ε_0 is called the permittivity of free space. (If q and Q have opposite signs, the repulsive barrier becomes an attractive well.)

de Broglie relationship (21) The relationship $\lambda = h/p$ between the *de Broglie wavelength* and the magnitude of momentum of a *free particle*.

de Broglie wave (20) A wave used in *quantum physics* to describe a *free particle*.

de Broglie wave function (27) The *wave function* $Ae^{i(kx-\omega t)}$ that describes a *stationary state* of a *free particle* in *quantum mechanics*.

de Broglie wavelength (21) The *wavelength* of a *de Broglie wave*, given by the *de Broglie relationship* $\lambda = h/p$.

decay constant (13) A quantity, λ, with units of inverse time, characterizing radioactive decay in a specific kind of *nucleus* (or other unstable particle). The *probability* of decay in a short time interval δt is $\lambda\,\delta t$, which is independent of time. Given a large sample of nuclei of the same kind, the average number of nuclei that remain undecayed at time t falls exponentially according to the law

$$N(t) = N(0)\,e^{-\lambda t}.$$

See also *half-life*.

degeneracy (81) The occurrence of different quantum *states* with the same energy.

degenerate (81) Two quantum *states* are said to be degenerate with one another if they have the same energy. An *energy level* that corresponds to more than one quantum state is also said to be degenerate.

dependent variable In a function $f(x, y, \ldots, z)$, the dependent variable is f. Contrast with *independent variables* $x, y, \ldots, z$.

destructive interference (30) The phenomenon in which two or more waves cancel one another when they are superimposed at a given point.

deterministic (13) A term indicating that identical initial conditions lead to identical outcomes on all occasions. Contrast with *indeterministic*.

deuteron (91) A *nucleus* consisting of a *proton* and a *neutron* bound together.

differential cross-section (196) A quantity used to measure the rate per unit incident *flux* per unit solid angle, at which a given type of target scatters a given type of incident particle into a small cone of angles around a specified direction.

differential equation (217) An equation that involves derivatives of a function. *Ordinary differential equations* involve ordinary derivatives, while *partial differential equations* involve *partial derivatives*. However, the term 'differential equation' is sometimes used as a shorthand for 'ordinary differential equation'. The process of solving the differential equation involves finding functions that satisfy the equation, subject to appropriate *boundary conditions* or *initial conditions*.

diffraction (16) The spreading of a wave that occurs when it passes through an aperture or around an obstacle. Classical examples include the diffraction of water waves, sound waves and light waves. In *quantum mechanics*, the wave could be the *wave function* that describes an *electron* propagating according to *Schrödinger's equation* after passing through a narrow slit.

diffraction pattern (18) The intensity pattern of a wave that has been diffracted by passing through an aperture or around an obstacle. The diffraction arises as a result of *interference*, so the diffraction pattern generally displays *interference maxima* and *interference minima*.

discrete set of values A set of values is said to be discrete if any two distinct values are separated by a finite gap.

Ehrenfest's theorem (158) This theorem states that the *expectation values* of the position and momentum of a single particle obey the equations

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p_x\rangle}{m}$$

and

$$\frac{d\langle p_x\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x}\right\rangle,$$

where V is the *potential energy function*. Ehrenfest's theorem is always true. In the *classical limit*, it helps us to understand how the results of *quantum mechanics* approach those of *classical mechanics*.

eigenfunction (43, 221) A function that satisfies an *eigenvalue equation* together with appropriate *boundary conditions*. In *wave mechanics*, *energy eigenfunctions* with different *eigenvalues* are mutually *orthogonal*.

eigenvalue (43, 221) A value of the parameter λ that appears in the *eigenvalue equation* $\widehat{A}f(x) = \lambda f(x)$ and is consistent with the given *boundary conditions*.

eigenvalue equation (43, 221) In the context of functions of a single variable, an eigenvalue equation is an equation of the form $\widehat{A}f(x) = \lambda f(x)$, where $\widehat{A}$ is an *operator*, and the constant λ is an undetermined parameter. In many cases, the acceptable solutions of such an equation are required to satisfy *boundary conditions* (for example, we may require them to remain finite as x approaches $\pm\infty$).

Any function that satisfies the eigenvalue equation (subject to appropriate boundary conditions) is called an *eigenfunction*, and the corresponding value of λ is called an *eigenvalue*. The prefix 'eigen' comes from the German for characteristic and indicates the 'special' nature of the eigenfunctions and eigenvalues of an operator. In a wide range of cases in *quantum mechanics*, the eigenvalues of an operator represent the only possible outcomes of a measurement of the corresponding *observable*.

elastic scattering (196) *Scattering* in which kinetic energy is conserved and particles do not change their nature or their state of internal excitation; nor are they created, destroyed or absorbed. Contrast with *inelastic scattering*.

electron A negatively-charged, spin-$\frac{1}{2}$ particle, currently regarded as structureless, with about one two-thousandth the mass of a *proton*.

electronvolt (11) A unit of energy defined as the energy gained when an *electron* is accelerated through a potential difference of 1 volt. An electronvolt is given the symbol eV, and is equal to 1.60×10^{-19} J. According to the conventional rules for SI prefixes, $1\,\text{meV} = 10^{-3}\,\text{eV}$, $1\,\text{keV} = 10^{3}\,\text{eV}$, $1\,\text{MeV} = 10^{6}\,\text{eV}$ and $1\,\text{GeV} = 10^{9}\,\text{eV}$. The units meV, eV, MeV and GeV are convenient for discussing molecular rotations, electronic transitions, nuclear physics and high-energy particle physics, respectively.

energy eigenfunction (56) An eigenfunction of the *Hamiltonian operator* for a given *system*.

energy eigenvalue (56) An eigenvalue of the *Hamiltonian operator* for a given *system*.

energy level (10) An energy that characterizes a particular *state* of a quantum *system*. In bound systems, such as nuclei, atoms and molecules, the energy levels are discrete. When such systems become unbound, as in the case of an *ionized* atom, the levels form a *continuum*. Do not confuse energy levels with the quantum states they characterize.

energy quantization (70) The quantum phenomenon in which *bound states* have discrete *energy levels*.

equation of continuity (189) An equation used in the description of fluid flow that relates changes in the density of fluid in any small region to the flow of fluid through the boundaries of that region. In *wave mechanics*, the *probability density* and *probability current density* obey a similar equation of continuity.

Euler's formula (214) The relationship

$$e^{i\theta} = \cos\theta + i\sin\theta$$

that links the exponential function to the cosine and sine functions.

even function (78) A function $f(x)$ for which $f(x) = f(-x)$ for all x.

expectation value (111, 229) For a given *random variable* A, the expectation value $\langle A\rangle$ is the theoretical prediction for the *average value* $\overline{A}$ in the limiting case of a large number of measurements.

Given a discrete set of possible outcomes, $A_1, A_2, \ldots$, with *probabilities* $p_1, p_2, \ldots$, the expectation value of A is given by

$$\langle A\rangle = p_1A_1 + p_2A_2 + \ldots = \sum_i p_iA_i,$$

where the sum runs over all the possible values for A.

For a random variable x with a continuous set of possible outcomes, the expectation value is given by

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

where $\rho(x)$ is the *probability density function* for the variable x.

In *quantum mechanics*, the expectation value of an *observable* A is the quantum-mechanical prediction for the average value of A when measurements are taken on a large number of identical *systems* all prepared in the same quantum *state*. In *wave mechanics*, the expectation value of any observable can be calculated by using the *sandwich integral rule*.

exponential form (214) A *complex number* is said to be expressed in exponential form if it is written as

$$z = re^{i\theta},$$

where r and θ are *real numbers* called respectively the *modulus* and the *phase* of z. Any complex number can be expressed in this way.

F-centre (83) A defect in an *ionic crystal* (such as NaCl) in which an ejected negative *ion* is replaced by an *electron* that acts as a particle trapped in a three-dimensional box created by the surrounding ions. F-centres can absorb one or more *wavelengths* of visible light; if present in sufficient numbers, they can alter the colour of a crystal.

finite square barrier (181) In one dimension, a *potential energy function* characterized by a constant value of potential energy (usually positive) over some finite continuous region of space, with a smaller constant value (usually zero) elsewhere.

finite square step (184) In one dimension, a *potential energy function* characterized by a constant value of potential energy over some semi-infinite region of space, with a different constant potential energy elsewhere.

finite square well (85) In one dimension, a *potential energy function* that has a finite constant value (often chosen to be zero) everywhere except for a finite region of length L. Within that region the potential energy has a lower constant value (often chosen to be negative). The concept may be generalized to two and three dimensions.

finite well (56) Any member of a class of *potential energy functions* which are finite everywhere, possess a local minimum, and approach a constant value (usually taken to be zero) at large distances from the minimum.

first-order partial derivative (224) A function obtained by taking the *partial derivative* of a given function.

flux (196) A quantity that describes the rate of flow of particles around a given point in three-dimensional space. The flux is the rate of flow of particles, per unit time per unit area, through a tiny area centred on the given point and perpendicular to the direction of flow of particles at the point. The SI unit of flux is the $\mathrm{m^{-2}\,s^{-1}}$.

force constant (125) The positive constant C that appears in *Hooke's law*, $F_x = -Cx$, and in the expression for the *potential energy function* of a *harmonic oscillator*, $V(x) = \frac{1}{2}Cx^2$. The SI unit of a force constant is $\mathrm{N\,m^{-1}}$.

Fourier transform (171) The Fourier transform $A(k)$ of a function $f(x)$ is defined by

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x.$$

The *momentum amplitude*, $A(k)$, of a *free particle* is the Fourier transform of the initial *wave function*, $\Psi(x, 0)$. See also *inverse Fourier transform*.

free particle (166) A particle that is not subject to forces, i.e. one for which the *potential energy function* is independent of position. It is conventional to take the potential energy of a free particle to be equal to zero, so the *Hamiltonian operator* for a free particle contains no potential energy term.

frequency (17) The number of cycles per unit time of an oscillation or wave. The frequency f is related to the *period* T by $f = 1/T$. The SI unit of frequency is the *hertz* (Hz) with $1\,\mathrm{Hz} = 1\,\mathrm{s^{-1}}$.

fusion reaction (205) A nuclear reaction in which low-mass nuclei combine to form a *nucleus* with a lower mass than the total mass of the nuclei that fused to form it. Fusion reactions are accompanied by the release of energy and often proceed by quantum-mechanical *tunnelling*.

Gaussian function (131) A function of the form

$$f(x) = C_0\mathrm{e}^{-x^2/2a^2},$$

where C_0 and a are constants. The *energy eigenfunctions* of a *harmonic oscillator* all involve Gaussian functions.

Gaussian wave packet (182) A *wave packet* in which $|\Psi|^2$ is shaped like a *Gaussian function* (for a suitable choice of origin).

Geiger counter (19) A device for detecting particles that are able to *ionize* molecules in a gas. Also called a Geiger–Müller tube.

Geiger–Nuttall relation (203) A relation linking the *decay constant* λ of a *nucleus* that emits *alpha particles* to the alpha-particle emission energy E_α of that nucleus. The relation applies to specific families of nuclei (such as *isotopes* of a given nucleus) and may be written in the form $\lambda = A\mathrm{e}^{-B/E_\alpha^{1/2}}$ where A is a constant that characterizes the particular family of nuclei, and B depends on the charge of the individual nucleus.

general solution of a differential equation (218) An expression that describes the general family of functions that satisfy the *differential equation*. The general solution of a differential equation of *order* n contains n *arbitrary constants*.

ground state (10) The *state* of lowest energy in a given quantum *system*. In the case of a system that displays *degeneracy*, there may be more than one such state.

half-life (14) For a given type of *nucleus*, the time $T_{1/2}$ over which half of the nuclei, on average, decay. The half-life is related to the *decay constant* λ by $T_{1/2} = \ln 2/\lambda$.

half-silvered mirror (15) A mirror coated in such a way that if many *photons* fall on any part of it, at an angle of incidence of $45°$, half are transmitted and half are reflected. A *half-silvered mirror* is an example of a *beam splitter*.

Hamiltonian function (47) A function which, in *classical mechanics*, expresses the total energy of a system as a sum of (i) the kinetic energy expressed in terms of momentum, and (ii) the *potential energy function* of the system.

Hamiltonian operator (48) The *operator* corresponding to the total energy of a *system*, obtained from the classical *Hamiltonian function* of the system by replacing each *observable* by the corresponding quantum-mechanical *operator*. See also *Schrödinger's equation* and *time-independent Schrödinger equation*.

harmonic oscillator (124) A *system* described by a classical *Hamiltonian function* of the form

$$H = \frac{p_x^2}{2m} + \tfrac{1}{2}Cx^2 = \frac{p_x^2}{2m} + \tfrac{1}{2}m\omega_0^2x^2,$$

where m is the mass of the oscillating particle, C is the *force constant* and ω_0 is the *angular frequency*.

In *wave mechanics*, a harmonic oscillator obeys the *Schrödinger equation*

$$\mathrm{i}\hbar\,\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\,\frac{\partial^2\Psi}{\partial x^2} + \tfrac{1}{2}m\omega_0^2x^2\,\Psi(x,t)$$

where ω_0 is now called the classical angular frequency.

Heisenberg uncertainty principle (117) This principle asserts that, in all *systems* and all *states*, the *uncertainties* in position and momentum of a particle obey the inequality

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

where $\hbar$ is *Planck's constant* h divided by 2π.

Hermite polynomial (134) A polynomial $H_n(x/a)$ that appears in the *energy eigenfunctions* of a *harmonic oscillator*:

$$\psi_n(x) = C_n H_n(x/a)\,\mathrm{e}^{-x^2/2a^2},$$

where a is the *length parameter* of the oscillator and C_n is a *normalization constant*.

The nth-order Hermite polynomial is defined by

$$H_n(x) = \mathrm{e}^{x^2/2}\left(x - \frac{\mathrm{d}}{\mathrm{d}x}\right)^n \mathrm{e}^{-x^2/2} \quad \text{for } n = 0, 1, 2, \ldots.$$

hertz The SI unit of *frequency*, given the symbol Hz and equal to the inverse second: $1\,\mathrm{Hz} = 1\,\mathrm{s}^{-1}$.

homogeneous differential equation (218) A *differential equation* in which each term is proportional to the *dependent variable* or one of its derivatives with respect to the *independent variable*, and there is no term that is a constant or that depends only on the independent variable.

Hooke's law (125) The force F_x on a particle is said to obey Hooke's law if it is a *restoring force* (always acting towards the equilibrium position) and is proportional to the displacement of the particle from the equilibrium position. We write

$$F_x = -Cx,$$

where x is the displacement from equilibrium, and the proportionality constant C is called the *force constant*. In *classical physics*, such a force leads to *simple harmonic motion*.

hyperbolic functions (220) Functions that involve certain combinations of e^x and e^{-x}. For each trigonometric function involving a given combination of $\mathrm{e}^{\mathrm{i}x}$ and $\mathrm{e}^{-\mathrm{i}x}$, there corresponds a hyperbolic function with the same combination of e^x and e^{-x}. The hyperbolic cosine and hyperbolic sine functions are:

$$\cosh x = \frac{\mathrm{e}^x + \mathrm{e}^{-x}}{2}$$

$$\sinh x = \frac{\mathrm{e}^x - \mathrm{e}^{-x}}{2}$$

imaginary axis (212) An axis in the *complex plane* on which the *real part* of *complex numbers* is equal to zero, and which points in the direction of increasing *imaginary part*.

imaginary number (210) A *complex number* of the form $\mathrm{i}y$, where y is real. Compare with *imaginary part*.

imaginary part (210) Given a *complex number* $z = x + \mathrm{i}y$, where x and y are *real numbers*, the imaginary part of z is equal to y. This is given by

$$y = \mathrm{Im}(z) = \frac{z - z^*}{2\mathrm{i}},$$

where z^* is the *complex conjugate* of z. Note that the imaginary part of a complex number is a real number and does not include a factor of i.

independent variable In a function $f(x, y, \ldots, z)$, the independent variables are $x, y, \ldots, z$. Contrast with *dependent variable* f.

indeterministic (13) A term indicating that identical initial conditions determine only the *probability* of specific outcomes rather than guaranteeing an identical outcome on all occasions. Contrast with *deterministic*.

inelastic scattering (196) *Scattering* for which the kinetic energy is not conserved. In inelastic scattering, particles may change their internal state of excitation or be absorbed; they may even be created or destroyed, especially at very high energies. Contrast with *elastic scattering*.

inertial frame (127) A reference frame in which any *free particle* has zero acceleration. Newton's laws are true only in an inertial frame.

infinite square well (65) In one dimension, a *potential energy function* that is infinite everywhere except for a finite region of length L. Within that region the potential energy has a constant value (which is usually taken to be zero.) The concept may be generalized to regions of any shape in two and three dimensions; the 'squareness' refers to the abrupt discontinuity in the potential energy function not to the shape of the region in space.

initial conditions (221) Conditions that supply extra information about the solution of a *differential equation* at a single value of the *independent variable*.

intensity of a beam (183) For one-dimensional *scattering* and *tunnelling* of a beam of particles, the (beam) intensity is the number of beam particles that pass a given point per unit time. The intensity of a beam can be identified with the magnitude of the corresponding *probability current*.

interference (16) The phenomenon arising from the superposition of two or more waves, resulting in a pattern of *interference maxima and minima*.

interference maxima (18) Features of *interference patterns* produced when two or more waves interfere with one another. Interference maxima occur at points where the contributing waves reinforce one another, leading to a local maximum in the intensity of the wave (*constructive interference*).

interference minima (18) Features of *interference patterns* produced when two or more waves interfere with one another. Interference minima occur at points where the contributing waves cancel one another, leading to a local minimum in the intensity of the wave (*destructive interference*).

interference pattern (18) The intensity pattern produced when two or more waves interfere with one another. See *interference*.

interference rule (32) A rule stating that, if a given process, leading from an initial *state* to a final state, can proceed in two or more alternative ways, and the way taken is not recorded, the *probability amplitude* for the process is the sum of the probability amplitudes for the different ways. When calculating the *probability* of the process, it is essential to add all the contributing probability amplitudes before taking the square of the *modulus*.

inverse Fourier transform (171) An operation which is the inverse of the *Fourier transform*. The inverse Fourier transform $f(x)$ of function $A(k)$ is defined as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, \mathrm{e}^{\mathrm{i}kx}\, \mathrm{d}k.$$

The initial *wave function* $\Psi(x,0)$ of a *free particle* is the inverse Fourier transform of the *momentum amplitude* $A(k)$.

ion (12) An electrically-charged atom that has lost or gained *electrons* so that the magnitude of its total electronic charge is not equal to the magnitude of the total charge of the *nucleus*.

ionic crystal (83) A crystal composed of negative and positive *ions* held together by the electrostatic attraction between ions of opposite sign. A well-known example is the crystal of common salt, NaCl.

ionization (12) The process in which a neutral atom loses one or more *electrons* to produce a positive *ion* and one or more unbound electrons.

ionized (11) The condition of an atom that has lost one or more *electrons*.

isotope (13) Different *nuclei* or atoms having the same *atomic number* Z, but different numbers N of *neutrons* and hence different *mass numbers* A are called isotopes of the element characterized by Z. The usual symbol for an isotope is $^{A}\mathrm{Sy}$, where Sy is the chemical symbol for the element and A is the mass number. Since Sy determines Z, the fuller notation $^{A}_{Z}\mathrm{Sy}$ is strictly redundant, but may be helpful for elements for which Z is not widely remembered. The full specification, $^{A}_{Z}\mathrm{Sy}_{N}$ is sometimes given, where N is the number of neutrons in the nucleus.

kinetic energy operator (44) The quantum mechanical *operator* representing the kinetic energy of a *system*. For a single particle in one dimension, the kinetic energy operator is

$$\widehat{\mathrm{E}}_{\mathrm{kin}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

Kronecker delta symbol (103) The symbol δ_{ij} that represents 1 if $i = j$, and represents 0 if $i \neq j$.

ladder operator (140) A term used to describe the *raising operator* or the *lowering operator* of a *harmonic oscillator*.

length parameter (133) For a *harmonic oscillator*, the length parameter is

$$a = \sqrt{\frac{\hbar}{m\omega_0}},$$

where m is the mass of the oscillating particle, $\omega_0 = \sqrt{C/m}$ is the classical *angular frequency* and C is the *force constant* of the oscillator. The length parameter characterizes the quantum properties of the oscillator.

linear combination (52) Given a set of functions $f_1(x)$, $f_2(x)$, ..., and a set of (possibly complex) constants c_1, c_2, ..., any expression of the form

$$c_1 f_1(x) + c_2 f_2(x) + \ldots$$

is called a linear combination of $f_1(x)$, $f_2(x)$, ...

linear differential equation (217) An *ordinary differential equation* of the form

$$\widehat{\mathrm{L}}y(x) = f(x),$$

where $\widehat{\mathrm{L}}$ is a *linear differential operator*.

linear differential operator (218) An *operator* of the form

$$\widehat{\mathrm{L}} = a_n(x)\frac{\mathrm{d}^n}{\mathrm{d}x^n} + a_{n-1}(x)\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}} + \ldots + a_1(x)\frac{\mathrm{d}}{\mathrm{d}x} + a_0(x),$$

where $a_n(x), a_{n-1}(x) \ldots a_0(x)$ are functions of x (some of which may be constant or equal to zero). A *linear differential equation* can be written in the form $\widehat{\mathrm{L}}y(x) = f(x)$ and *eigenvalue equations* can be written as $\widehat{\mathrm{L}}y(x) = \lambda y(x)$.

linear homogeneous differential equation (218) A *linear differential equation* in which each term is proportional to the *dependent variable* or one of its derivatives with respect to the *independent variable*, and there is no term that is a constant or that depends only on the independent variable.

linear number density (183) A quantity used to describe the number of particles per unit length, along a specified line. The SI unit of linear number density is m^{-1}.

linear operator (41) An *operator* $\widehat{\mathrm{O}}$ that satisfies the condition

$$\widehat{\mathrm{O}}(\alpha f(x) + \beta g(x)) = \alpha\widehat{\mathrm{O}}f(x) + \beta\widehat{\mathrm{O}}g(x)$$

for arbitrary complex constants α and β.

lowering operator (137) An *operator* $\widehat{\mathrm{A}}$ that, for $n \geq 1$, converts an *energy eigenfunction* $\psi_n(x)$ of a *harmonic oscillator* into the next eigenfunction of lower energy and for which $\widehat{\mathrm{A}}\psi_0(x) = 0$. If the eigenfunctions are *normalized*,

$$\widehat{\mathrm{A}}\,\psi_n(x) = \sqrt{n}\,\psi_{n-1}(x).$$

See also *raising operator* and *ladder operator*.

Mach–Zehnder interferometer (32) An arrangement of two *half-silvered mirrors*, which act as *beam splitters*, two fully reflecting mirrors, and two detectors, which is used to demonstrate *interference* phenomena in light.

mass number The total number of *protons* and *neutrons* in a *nucleus*, $A = N + Z$, where N is the number of neutrons and Z is the number of *protons* (the *atomic number*).

Maxwell's equations (17) A set of four *partial differential equations* relating the electric field $\mathbf{E}(\mathbf{r}, t)$ and magnetic field $\mathbf{B}(\mathbf{r}, t)$ to each other and to their sources in charges and currents. These are the basic field equations of classical electromagnetism.

mean value (111, 228) An alternative term for an *average value*.

modulus (210) The modulus $|z|$ of a *complex number* $z = x + \mathrm{i}y$ is a non-negative *real number* given by

$$|z| = \sqrt{x^2 + y^2},$$

where x and y are the *real part* and *imaginary part* of z. If the complex number is written in *polar form* $z = r(\cos\theta + \mathrm{i}\sin\theta)$ or in *exponential form* $z = r\mathrm{e}^{\mathrm{i}\theta}$, the modulus is equal to r.

momentum amplitude (170) A quantity whose *modulus* squared gives the *probability distribution* of momentum via *Born's rule for momentum*.

For a *free particle* in one dimension, the momentum amplitude $A(k)$ is the function that appears in the expansion of a free-particle *wave function* $\Psi(x, t)$ in terms of *de Broglie wave functions*:

$$\Psi(x, t) = \int_{-\infty}^{\infty} A(k)\, \mathrm{e}^{\mathrm{i}(kx - E_k t/\hbar)}\, \mathrm{d}x.$$

For non-free particles, the momentum amplitude $A(k, t)$ depends on time and is given by the *Fourier transform* of the wave function. Also called the *momentum wave function*.

momentum eigenfunction (168) For a single particle in one dimension, an *eigenfunction* of the *momentum operator* conventionally represented as

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}kx},$$

where k is a real constant called the *wave number* and the factor $1/\sqrt{2\pi}$ is included to simplify other equations in *quantum mechanics*. The corresponding momentum eigenvalue is $\hbar k$.

momentum operator (44) The quantum mechanical *operator* representing the momentum of a *system*. For a single particle in one dimension, the momentum operator is

$$\widehat{\mathrm{p}}_x = -\mathrm{i}\hbar\frac{\partial}{\partial x}.$$

momentum wave function (170) Another term for the *momentum amplitude*. In one dimension, this is written as $A(k)$.

mutually exclusive outcomes (228) A set of outcomes is said to be mutually exclusive if the occurrence of one of them in a given measurement implies that none of the others occur in that measurement. The *probability* that one or other of a set of mutually exclusive outcomes will occur is found by adding their individual probabilities. See the *addition rule for probability*.

neutron An electrically neutral constituent of the atomic *nucleus*, having a mass slightly greater than that of a *proton*.

nodes (73) Fixed points of zero disturbance in a *standing wave* (excluding points on the boundaries of the region where the disturbance takes place).

non-degenerate (100) A set of *stationary states* or *energy eigenfunctions* is said to be non-degenerate if all members of the set correspond to different energies.

normal ordering (138) The conventional order $\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}$ for the *raising* and *lowering operators* of a *harmonic oscillator*. These *operators* do not *commute* with one another. In fact, $\widehat{\mathrm{A}}\,\widehat{\mathrm{A}}^\dagger - \widehat{\mathrm{A}}^\dagger\,\widehat{\mathrm{A}} = \widehat{\mathrm{I}}$, where $\widehat{\mathrm{I}}$ is the *unit operator*. $\widehat{\mathrm{A}}^\dagger$

normalization condition (50) The condition, based on *Born's rule*, that requires a total *probability* of 1 for finding a given particle to be somewhere in the whole of space. For a single particle in one dimension, in a *state* described by the *wave function* $\Psi(x, t)$, the normalization condition takes the form

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2\, \mathrm{d}x = 1.$$

A similar condition applies to systems in more than one dimension.

Energy eigenfunctions $\psi_n(x)$ are also taken to obey a normalization condition:

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2\, \mathrm{d}x = 1.$$

normalization constant (50) A constant A chosen so that, if Φ is a *wave function*, then $\Psi = A\Phi$ is a *normalized* wave function. Due to the physical irrelevance of any overall *phase factor* multiplying a wave function, the normalization constant of a one-dimensional system may be taken to be the real positive constant

$$A = \left(\int_{-\infty}^{\infty} |\Phi(x, t)|^2\, \mathrm{d}x\right)^{-1/2}.$$

This turns out to be independent of time. This result can be extended to *energy eigenfunctions* and to systems in more than one dimension.

normalization rule (228) Given a *complete set* of discrete, *mutually exclusive outcomes*, their *probabilities* p_i obey the rule

$$\sum_i p_i = 1,$$

where the sum is over all outcomes in the set.

This condition can be extended to a variable x whose possible mutually exclusive outcomes form a continuum. In this case,

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

where $\rho(x)$ is the *probability density function* for the variable x.

normalized (50) A term used to describe a *wave function* or *eigenfunction* that satisfies the *normalization condition*.

nucleus The positively charged, very compact central part of an atom. The nucleus is some 10^4 times smaller in radius than an atom, and contains almost all the mass, the *protons* and *neutrons* of which it is composed each being some 2000 times more massive than an *electron*. The number of positively-charged protons, the *atomic number*, Z, determines the number of *electrons* in a neutral atom and hence the chemical properties of that element.

number operator (141) The *operator* $\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}$, where $\widehat{\mathrm{A}}^\dagger$ is the *raising operator* and $\widehat{\mathrm{A}}$ is the *lowering operator* for a *harmonic oscillator*. When the number operator acts on an *energy eigenfunction* of the harmonic oscillator, it gives the *eigenvalue equation*

$$\widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}}\,\psi_n(x) = n\,\psi_n(x),$$

where n is the *quantum number* of the eigenfunction $\psi_n(x)$.

observable (44) An attribute of a *system* that can, at least in principle, be measured by a specific experimental procedure. For a system consisting of a particle with a given *potential energy function*, the observables include the position, momentum and energy of the particle.

odd function (78) A function $f(x)$ for which $f(x) = -f(-x)$ for all x.

old quantum theory (7) A term given to attempts made between 1900 and 1925 to reconcile quantum concepts with *classical physics*. The resulting theory was based on ad-hoc ideas and never became a comprehensive world-view. While it had successes (explaining the *spectral lines* of hydrogen atoms) it ran into serious difficulties (failing to explain the spectral lines of helium atoms, for example). Old quantum theory was superseded by *quantum mechanics* in the period from 1924 to 1927.

one-dimensional infinite square well (65) See *infinite square well*.

operator (40) In the context of *wave mechanics*, an operator is a mathematical entity that acts on a function to produce another function. It is conventional to indicate an operator by putting a hat on it, as in $\widehat{\mathrm{O}}$. In *quantum mechanics* each *observable* has a corresponding *linear operator*. Examples of such operators include the *momentum operator* $\widehat{\mathrm{p}}_x = -\mathrm{i}\hbar\partial/\partial x$, the *position operator* $\widehat{\mathrm{x}} = x$ and the *Hamiltonian operator* $\widehat{\mathrm{H}}$, which is the operator for the total energy of a *system*.

order of a derivative The number of times the *dependent variable* of the derivative is differentiated with respect to the *independent variable*. For example, $\mathrm{d}^n y/\mathrm{d}x^n$ is a derivative of order n.

order of a differential equation (217) The *order* of the highest derivative that appears in the equation.

ordinary differential equation (217) A *differential equation* that involves only ordinary derivatives (and no *partial derivatives*). Sometimes, for brevity, called a differential equation.

orthogonal functions (102) Two functions $f(x)$ and $g(x)$ are said to be orthogonal if their *overlap integral* vanishes. That is,

$$\int_{-\infty}^{\infty} f^*(x)\,g(x)\,\mathrm{d}x = 0.$$

orthonormal set of functions (103) A set of functions $\psi_1(x), \psi_2(x), \ldots$ is said to be orthonormal if

$$\int_{-\infty}^{\infty} \psi_i^*(x)\,\psi_j(x)\,\mathrm{d}x = \delta_{ij}$$

where δ_{ij} is the *Kronecker delta symbol*.

overlap integral (101) The overlap integral of two functions $f(x)$ and $g(x)$ is given by

$$\int_{-\infty}^{\infty} f^*(x)\,g(x)\,\mathrm{d}x.$$

Overlap integrals are used to calculate *probability amplitudes* in *wave mechanics*.

overlap rule (101) For a system with discrete non-degenerate *energy eigenvalues* $E_1, E_2, \ldots$, the overlap rule states that the *probability* of obtaining the ith eigenvalue E_i is

$$p_i = \left|\int_{-\infty}^{\infty} \psi_i^*(x)\,\Psi(x,t)\,\mathrm{d}x\right|^2,$$

where $\psi_i(x)$ is the *normalized energy eigenfunction* with eigenvalue E_i, and $\Psi(x,t)$ is the normalized *wave function* describing the *state* of the system at the time of measurement. The integral between the *modulus* signs is called the *overlap integral* of $\psi_i(x)$ and $\Psi(x,t)$.

This rule can be extended to other *observables* with discrete eigenvalues, provided that the energy eigenfunctions are replaced by the eigenfunctions of the corresponding quantum-mechanical *operator*.

partial derivative (222) The partial derivative of a function $f(x, y, \ldots)$ of more that one variable with respect to the variable x is the derivative obtained by differentiating f with respect to x while treating all the other variables as constants.

partial differential equation (224) An equation that involves *partial derivatives* of an unknown function. See also *differential equation*.

partial differentiation (223) The process of differentiating a function of two or more variables with respect to one of its variables, while treating all the other variables as constants.

particular solution of a differential equation (218) A specific function that satisfies the *differential equation*. A particular solution is obtained from the *general solution* of the differential equation by selecting particular values of its *arbitrary constants*. The choice is usually made by imposing some additional physical restraints (*boundary conditions* or *initial conditions*).

period (17) The time T taken for one complete cycle of an oscillation or wave; the reciprocal of the *frequency*, $T = 1/f$.

phase (18, 213) For a sinusoidal *plane wave* $u(x, t) = A\cos(kx + \omega t + \phi)$, or a *simple harmonic oscillation* $u(t) = A\cos(\omega t + \phi)$, where A is positive, the phase is the argument of the cosine. Do not confuse the phase with the *phase constant*.

For a *complex number* written in *polar form* or in *exponential form*:

$$z = r(\cos\theta + \mathrm{i}\sin\theta) = r\mathrm{e}^{\mathrm{i}\theta},$$

the phase of the complex number is the *real number* θ (also called the *argument of the complex number*).

phase constant (18, 126) For a sinusoidal *plane wave* $u(x, t) = A\cos(kx + \omega t + \phi)$, where A is positive, the phase constant is ϕ.

phase factor (52, 214) A *complex number* of the form $\mathrm{e}^{\mathrm{i}\alpha}$, where α is real. The *modulus* of a phase factor is equal to 1. Multiplying a *wave function* by an overall phase factor has no physical significance.

photon (10) A packet of electromagnetic radiation. Photons are subject to *wave–particle duality*, with individual photons characterized by energy $E = hf = \hbar\omega$ and momentum magnitude $p = hf/c = \hbar\omega/c$ where f is the *frequency* and ω the *angular frequency* of the radiation.

Plancherel's theorem (169) A mathematical theorem which states that

$$\int_{-\infty}^{\infty} |\Psi(x, 0)|^2 \,\mathrm{d}x = \int_{-\infty}^{\infty} |A(k)|^2 \,\mathrm{d}k,$$

where $A(k)$ is the *Fourier transform* of $\Psi(x, 0)$. This theorem allows us to construct *normalized wave packets* for *free particles*, and underpins the interpretation of $A(k)$ as a *momentum amplitude*. Plancherel's theorem is sometimes inaccurately called Parseval's theorem.

Planck's constant (10) A fundamental constant $h = 6.63 \times 10^{-34}$ J s, which characterizes most quantum phenomena. The quantity $h/2\pi$ is given the symbol $\hbar$.

plane wave A wave in which points of constant *phase* lie in planes perpendicular to the direction of propagation of the wave.

polar coordinates A pair of coordinates r and θ used to specify the position of a point in a plane. Polar coordinates are related to Cartesian coordinates (x, y) by

$$x = r\cos\theta, \quad \text{and} \quad y = r\sin\theta.$$

The radial coordinate is given by $r = \sqrt{x^2 + y^2}$ and the angular coordinate is found by solving either $\tan\theta = y/x$ or $\cos\theta = x/r$ for θ, taking care to choose an angle in the appropriate quadrant.

polar form (213) The polar form of a *complex number* is

$$z = r(\cos\theta + \mathrm{i}\sin\theta),$$

where r is the *modulus* of the complex number and θ is its *phase* or *argument*. The modulus lies in the range $0 \le r < \infty$. It is always possible to add any integer multiple of 2π to the phase without changing the complex number.

position operator (45) The quantum-mechanical *operator* representing the position of a particle. In one dimension, the position operator is $\widehat{\mathrm{x}} = x$; that is, the operation of multiplying a function $f(x)$ by the variable x.

potential energy function (46) A function describing the potential energy of a system. Examples include the *free-particle* potential energy function which is a constant (usually taken to be zero) everywhere, the one-dimensional *harmonic oscillator* potential energy function $V(x) = \frac{1}{2}Cx^2$, and various *finite well* potential energy functions.

potential energy operator (45) The quantum mechanical *operator* representing the potential energy of a system. For a single particle in one dimension, the potential energy operator is $\widehat{\mathrm{V}} = V(x)$; that is, the operation of multiplying a function $f(x)$ by the *potential energy function* $V(x)$.

principle of superposition (52, 219) The property of a *linear homogeneous differential equation* whereby, if $y_1(x)$ and $y_2(x)$ are solutions of the differential equation, then so is the *linear combination* $c_1y_1(x) + c_2y_2(x)$, where c_1 and c_2 are any constants. *Schrödinger's equation* is a *linear homogeneous* *partial differential equation*, so the principle of superposition applies to it.

probabilistic (13) An alternative term for *indeterministic*.

probability (227) A number between 0 and 1 used to quantify the likelihood of an uncertain outcome, with larger probabilities corresponding to more likely outcomes; impossibility is represented by 0 and certainty by 1.

probability amplitude (31, 102) A quantity that emerges from quantum-mechanical calculations and refers to a given experimental outcome. The *probability* of the experimental outcome is obtained by taking the square of the *modulus* of the probability amplitude. Probability amplitudes obey the *interference rule*. In *wave mechanics*, probability amplitudes can be calculated using the *overlap rule* or the *coefficient rule*.

probability current (190) A signed quantity that describes the rate of flow of *probability density* in one dimension. For a particle of mass m, or a beam of particles each of mass m, the probability current is defined by the relation

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

where $\Psi(x,t)$ is the *wave function* describing the particle or beam. The SI unit of probability current is s^{-1}.

probability density (50) For a particle in one dimension, in a *state* described by the *wave function* $\Psi(x,t)$, the probability density is given by $|\Psi(x,t)|^2$. This is the *probability* per unit length of finding the particle in a small interval centred on x.

A similar definition applies in three dimensions, where the probability density $|\Psi(\mathbf{r},t)|^2$ is the probability per unit volume of finding the particle in a small region centred on $\mathbf{r}$.

Strictly speaking, the probability density is correctly called the *probability density function* for position.

probability density function (232) For any continuous *random* variable, a, the probability density function is a function $\rho(a)$, defined such that the *probability* of obtaining a value of a lying in a small range of width δa, centred on a_0 is $\rho(a_0)\,\delta a$. The probability P of finding a value of a between a_1 and a_2 is

$$P = \int_{a_1}^{a_2} \rho(a)\,\mathrm{d}a.$$

The probability density function satisfies the *normalization condition*

$$\int_{-\infty}^{\infty} \rho(a)\,\mathrm{d}a = 1.$$

The probability density function for position is often referred to simply as the *probability density*.

probability distribution (229) For a discrete *random* variable, a function that assigns a *probability* to each possible value of the variable. For a continuous random variable, a function that assigns a *probability density* to each possible value of the variable.

proton A positively-charged constituent of atomic *nuclei*, having a mass almost 2000 times that of an *electron*, and a positive charge with the same magnitude as a negatively-charged electron.

proton–proton chain (206) A sequence of nuclear reactions found in stars like the Sun that have the net effect of converting hydrogen to helium.

quantization (10) The fact that the measured values of some *observable* quantities have a discrete set of allowed values (in given *systems*, over given ranges).

quantum dot (63) An artificially-created structure in which a tiny ‘speck’ of one *semiconducting material* is entirely embedded in a larger sample of another semiconducting material. The embedded speck is typically a few nanometres across. Such a structure can be modelled as a microscopic three-dimensional box in which *electrons* can be confined.

quantum mechanics (7) A term given to the comprehensive quantum theory of *systems* of finite numbers of particles that superseded *old quantum theory* and *classical mechanics*. Quantum mechanics has both non-relativistic and relativistic branches. However, it does not cover systems in which particles are created or destroyed: that is the province of quantum field theory. This course focuses on the non-relativistic aspects of quantum mechanics.

quantum number (57) A discrete index (often an integer) used to label an *eigenfunction*, *eigenvalue*, *wave function* or quantum *state*.

A single quantum number may be enough to specify a state in a one-dimensional system. An example is the quantum number n that specifies a particular state of a particle in a *one-dimensional infinite square well*, with $n = 1$ specifying the *ground state*. At least three quantum numbers are needed to fully specify a *state* in three-dimensional systems.

quantum physics (7) A term given to any branch of physics that is based on quantum ideas. For example, aspects of nuclear physics, atomic physics or solid-state physics may be classified as being quantum physics.

quantum random number generator (15) A device that uses the fundamental *indeterminism* of *quantum mechanics* to generate a sequence of *random* numbers.

quantum wafer (64) An artificially-created structure in which a thin layer of one *semiconducting material* is sandwiched between thicker layers of another semiconducting material. The thin layer is typically a few nanometres thick. Such a structure allows *electrons* to move freely in two dimensions while being narrowly confined in the third.

quantum wire (63) An artificially-created structure in which a thin 'thread' of one *semiconducting material* is embedded in another semiconducting material. The embedded thread is typically a few nanometres across. Such a structure allows *electrons* to move freely in one dimension while being narrowly confined in the other two dimensions.

radiative transition (145) A transition from one *energy level* to another that is accompanied by the absorption or emission of a *photon*.

raising operator (137) An *operator* $\widehat{\mathrm{A}}^\dagger$ that converts an *energy eigenfunction* $\psi_n(x)$ of a *harmonic oscillator* into the next energy eigenfunction of higher eigenvalue. If the eigenfunctions are *normalized*,

$$\widehat{\mathrm{A}}^\dagger \psi_{n-1}(x) = \sqrt{n}\,\psi_n(x).$$

See also *lowering operator* and *ladder operator*.

Ramsauer–Townsend effect (196) A sharp dip in the measured *total cross-section* for the *scattering* of *electrons* by noble gas atoms (such as xenon) at an energy of about 1 eV. This is a three-dimensional analogue of the *transmission resonance* found in one dimension.

random (227) A variable is said to be random if its possible values have definite *probabilities*, but no further information is available to us about which of its values will be obtained.

real axis (212) An axis in the *complex plane* on which the *imaginary part* of *complex numbers* is equal to zero, and which points in the direction of increasing *real part*.

real number (210) An ordinary number; in other words, a *complex number* with no *imaginary part*.

real part (210) Given a *complex number* $z = x + \mathrm{i}y$, where x and y are *real numbers*, the real part of z is equal to x. This is given by

$$x = \mathrm{Re}(z) = \frac{z + z^*}{2},$$

where z^* is the *complex conjugate* of z.

reduced mass (128) Observed from the centre-of-mass frame, the energy of a two-particle system takes the form of the energy of a single particle of reduced mass μ, subject to an external *potential energy function*. The reduced mass μ is given by

$$\mu = \frac{m_1 m_2}{m_1 + m_2},$$

where m_1 and m_2 are the masses of the two particles.

reflection coefficient (182) The *probability* that a specified one-dimensional *potential energy function* will cause an incident particle to reverse its direction of motion.

relative frequency (229) If a quantity A is measured N times and the result A_i is obtained on N_i occasions, the relative frequency of the result A_i is N_i/N.

restoring force (125) A force that acts in a direction that tends to restore a particle towards its equilibrium position.

sandwich integral (112) An integral of the form

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\widehat{\mathrm{A}}\,\Psi(x,t)\,\mathrm{d}x,$$

where $\widehat{\mathrm{A}}$ is a quantum-mechanical operator, used to calculate the *expectation value* of an *observable* A at time t.

sandwich integral rule (112) In a *state* described by the *wave function* $\Psi(x,t)$, the *expectation value* of an *observable* A is given by the *sandwich integral*

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\,\widehat{\mathrm{A}}\,\Psi(x,t)\,\mathrm{d}x,$$

where $\widehat{\mathrm{A}}$ is the quantum-mechanical *operator* corresponding to A. This rule is valid for all *observables*, whether their values are discrete or continuous.

scanning tunnelling microscope (STM) (206) A kind of microscope that produces atomic-scale maps of surface structure by monitoring the *tunnelling* of *electrons* through the small gap between a sample's surface and a very thin probe tip that is scanned across the surface.

scattering (178) A process in which an incident particle (or wave) is affected by interaction with some kind of target, quite possibly another particle. The interaction can affect the incident particle in a number of ways; it may change its speed, direction of motion or state of internal excitation. Particles can even be created, destroyed or absorbed. Scattering may be *elastic* or *inelastic*. In one dimension, scattering may be described in terms of the *reflection coefficient* and the *transmission coefficient*. More generally, it is described in terms of the *total cross-section* and the *differential cross-section*.

Schrödinger's equation (24, 46) The *partial differential equation* that governs the time development of the *wave function* Ψ describing the *state* of a *system* in *wave mechanics*. Schrödinger's equation may be written in the general form

$$\mathrm{i}\hbar\frac{\partial \Psi}{\partial t} = \widehat{\mathrm{H}}\Psi,$$

where $\widehat{\mathrm{H}}$ is the *Hamiltonian operator* and $\hbar = h/2\pi$, h being *Planck's constant*. In any specific situation $\widehat{\mathrm{H}}$ takes a form that characterizes the system under consideration, and Ψ depends on the possible coordinates of particles in the system as well as on time. For example, in the case of a one-dimensional system consisting of a particle with *potential energy function* $V(x)$, Schrödinger's equation takes the form

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

second-order partial derivative (224) A function obtained by partially differentiating another function twice (possibly with respect to different independent variables).

selection rule (131) A rule that selects *radiative transitions* between quantum *states* from a wider range of possibilities. For a *harmonic oscillator*, a selection rule restricts radiative transitions to those between neighbouring *energy levels*.

semiconducting materials (63) Materials such as silicon and germanium with an electrical conductivity intermediate between that of a conductor and that of an insulator.

separable partial differential equation (226) A *partial differential equation* for which the method of *separation of variables* produces an equation in which one of the variables appears on one side of the equation and does not appear on the other side of the equation.

separation constant (54, 226) An undetermined constant that appears when a *partial differential equation* is solved by the method of *separation of variables*. The separation constant then appears in the *eigenvalue equations* for the separated variables.

separation of variables (53, 225) A method used for finding some solutions of some *partial differential equations*. It involves expressing the solution as a product of functions of different *independent variables*, rewriting the original equation as a separated equation in which one side is independent of one of those independent variables, and then solving the two differential equations obtained by setting each side of the separated equation equal to a common *separation constant*.

In the case of *Schrödinger's equation* for a one-dimensional *system* consisting of a particle with a given *potential energy function* $V(x)$ that is independent of time, the solution $\Psi(x,t)$ may be written as the product $\psi(x)T(t)$, where $\psi(x)$ is a solution of the *time-independent Schrödinger equation* for the system, $T(t) = \mathrm{e}^{-\mathrm{i}Et/\hbar}$, and the separation constant E represents the total energy of the system.

simple harmonic motion (124) Motion that characterizes a *harmonic oscillator* in *classical physics*, in which the displacement of a particle depends sinusoidally on time.

simple harmonic oscillation Another term for *simple harmonic motion*.

simple harmonic oscillator (124) Another term for a *harmonic oscillator*.

sinusoidal function Any function of the form

$$f(x) = A\sin(x+\phi)$$

where A and ϕ are constants. Thus $\cos(x)$ and $\sin(x) + \cos(x)$ are sinusoidal functions.

spectra (9) The plural of *spectrum*.

spectral lines (9) Narrow lines (corresponding to narrow ranges of *wavelength*) seen in the *spectra* of substances and characteristic of those substances. Each spectral line has a *frequency* $f = \Delta E/h$, where ΔE is the difference in energy between two quantum *states* in the *system*.

spectrum (9) The pattern of *spectral lines* observed when light is emitted or absorbed by a quantum *system*. The spectrum can provide an identifiable 'fingerprint' of the system.

standard deviation (116, 230) A quantity that measures the amount by which a set of data values spreads out on either side of the *average value*. The standard deviation of a quantity A is defined as

$$\sigma(A) = \left[\ \overline{\left(A-\overline{A}\right)^2}\ \right]^{1/2},$$

where the bars indicate average values. As the number of data values tends to infinity, the standard deviation $\sigma(A)$ is expected to approach the *uncertainty* ΔA.

(Statisticians sometimes use a slightly different quantity called the sample standard deviation. This differs from our definition by an amount that becomes vanishingly small as the number of data values tends to infinity.)

standing wave (73) A wave that oscillates without travelling through space. All points in the disturbance that constitutes the wave oscillate in phase, with the same *frequency* but with different *amplitudes*. Various points of zero disturbance may be *nodes* of the wave. These nodes remain fixed in position.

A common example of a standing wave is a wave on a string stretched between fixed endpoints. In such a case the standing waves that may be excited are restricted by the requirement that the distance between the fixed ends of the string must be equal to a whole number of half-*wavelengths*. A *stationary-state wave function* in *quantum mechanics* describes a complex standing wave.

state (51) The condition of a *system* described in sufficient detail to distinguish it from other conditions in which the system would behave differently. In *classical mechanics*, the state of a system at a particular time can be completely specified by giving the values of a set of measurable quantities at that time. In *wave mechanics*, the state of a system at a particular time is specified by the *wave function* at that time. Everything that can be said about the *probabilities* of the outcomes of measurements is implicit in the wave function.

stationary state (57) A solution of *Schrödinger's equation* described by a *wave function* which is a product of a factor that depends on spatial coordinates and a factor that depends on time. In any stationary state the energy has a definite value and the *probability distribution* associated with any *observable* is independent of time. In one dimension, the *wave function* of a stationary state can be expressed as $\psi(x)\mathrm{e}^{-\mathrm{i}Et/\hbar}$, where E is the total energy of the system and $\psi(x)$ is a solution of the *time-independent Schrödinger equation* corresponding to the *energy eigenvalue* E.

superposition principle (52) See *principle of superposition*.

symmetric well (76) In one dimension, a well described by a *potential energy function* $V(x)$ that has the property $V(x) = V(-x)$. Symmetric wells have *energy eigenfunctions* that are either *even functions* or *odd functions*. The even or odd nature of eigenfunctions alternates with increasing energy.

system Part of the Universe that is singled out for study. We often consider isolated systems of particles, which are not subject to forces caused by agencies outside the system.

time-independent Schrödinger equation (55) An energy *eigenvalue equation* that can be derived from *Schrödinger's equation* for a *system* of particles interacting through a specified *potential energy function* in cases where the potential energy function is independent of time. The time-independent Schrödinger equation may be written in the form

$$\widehat{\mathrm{H}}\psi = E\psi,$$

where $\widehat{\mathrm{H}}$ is the (time-independent) *Hamiltonian operator*, ψ is an *energy eigenfunction* and E is the corresponding *energy eigenvalue*. In any specific situation $\widehat{\mathrm{H}}$ will take a form that characterizes the system under consideration. For example, in the case of a one-dimensional system consisting of a particle with potential energy function $V(x)$ the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x) = E\psi(x),$$

where $\hbar$ is *Planck's constant* divided by 2π.

total cross-section (196) A quantity used to measure the total rate per unit time per unit incident *flux*, at which a given type of target scatters a given type of incident particle. The SI unit of total cross-section is m^2 but the *barn* is a more commonly-used unit in particle and nuclear physics.

transmission coefficient (182) The *probability* that a specified one-dimensional *potential energy function* will allow an incident particle to pass, continuing in its original direction of motion.

transmission resonances (194) For one-dimensional scattering, a transmission resonance is a maximum in the *transmission coefficient* T as a function of energy, ideally with $T = 1$, corresponding to perfect transmission and no reflection.

tunnelling (179) The quantum-mechanical phenomenon in which incident particles, initially in a *classically allowed region*, are able to pass through a *classically forbidden region* and emerge on the far side of it, travelling in another classically allowed region. Tunnelling occurs in *alpha-particle decay*, *fusion reactions* in the *proton–proton chain* and the *scanning tunnelling microscope*.

two-slit interference pattern (18) The pattern of maxima and minima that forms when a *plane wave* is incident on an absorbing screen that contains two narrow slits. The pattern, formed on the far side of the absorbing screen, consists of a series of bright bands separated by dark bands. The bright bands occur in places where the waves passing through the two slits interfere constructively. The dark bands occur in places where these waves interfere destructively. The two slits must be narrow enough for their two *diffraction patterns* to appreciably overlap. This implies that their widths must be comparable to, or smaller than, the *wavelength* of the incident wave. See also *constructive interference* and *destructive interference*.

uncertainty (116, 231) The quantum-mechanical prediction for the *standard deviation* of an *observable* in a *system* in a given *state*. The uncertainty is defined by

$$\Delta A = \left[\left\langle (A - \langle A\rangle)^2 \right\rangle\right]^{1/2}$$

where $(A - \langle A\rangle)^2$ is the square of the deviation of A from its *expectation value*. Uncertainties can also be calculated from the formula

$$\Delta A = \left[\langle A^2\rangle - \langle A\rangle^2\right]^{1/2}.$$

Compare with *standard deviation*.

uncertainty principle (117) A shorthand term for the *Heisenberg uncertainty principle*.

unit operator An operator $\widehat{\mathrm{I}}$ that does not affect any function it acts on: $\widehat{\mathrm{I}}\,f(x) = f(x)$.

wave function (24, 49) A function that fully describes the *state* of a system in *wave mechanics*. For a single particle in one dimension, the wave function takes the form $\Psi(x, t)$. The wave function evolves in time according to *Schrödinger's equation*, except when the system is disturbed by a measurement, leading to the *collapse of the wave function*.

The spatial extent of a particle's wave function is not to be confused with the size of the particle. For example, the spatial extent of the wave function of an *electron* in an atom is the spatial extent of the atom, whilst the electron itself is much smaller, a point particle as far as we can tell.

wave mechanics (7) A term given to a way of formulating *quantum mechanics*, and carrying out quantum-mechanical calculations, pioneered by Erwin Schrödinger. In wave mechanics, the *state* of a system is described by a *wave function*, which obeys a *partial differential equation* called *Schrödinger's equation*. *Observable* quantities are represented by differential *operators* that act on the wave function.

wave number (17) A quantity $k = 2\pi/\lambda$ that describes a *plane wave*, where λ is the *wavelength* of the wave.

wave packet (150) A *wave function* that is a *linear combination* of two or more different *stationary-state* wave functions. Any wave function (other than one describing a stationary state) can normally be expressed in this way.

wave–particle duality (17) The phenomenon whereby *systems* display properties associated with both particles and waves according to the kind of measurements performed on them. It shows that it is best to think of 'particle' and 'wave' as categories associated with our macroscopic world; there is no obligation for microscopic entities to fall wholly into one category or the other.

wave-packet spreading (172) The phenomenon whereby a particle described by a *wave packet* has an *uncertainty* in position that changes (normally increases) with time.

wavelength (17) The spatial separation, λ, of successive points in a wave that differ in *phase* by 2π at any fixed time t. More crudely, the distance between successive peaks (or troughs) of the wave.

zero-point energy (130) The *ground-state* energy of a particle, measured from the bottom of its potential energy well. This energy would be present even at the absolute zero of temperature.