Glossary

angular node | An angular node will occur where the angular part of the electronic wavefunction equals zero.

ansatz | An educated guess or an additional assumption made to help solve a problem, and which is later verified to be part of the solution by its results.

atomic orbitals | Atomic orbital is a mathematical function describing the location and wave-like behavior of a single electron in an atom. This function can be used to calculate the probability of finding any electron of an atom in any specific region around the atom's nucleus.

Beer's Law | The Beer-Lambert law relates the optical attenuation of a physical material containing a single attenuating species of uniform concentration to the optical path length through the sample and absorptivity of the species.

Bohr magneton | A physical constant and the natural unit for expressing the magnetic moment of an electron caused by either its orbital or spin angular momentum. ($\mu_B = e\hbar/2m_e$)

Bosons | Bosons are particles with integer spin (s = 0, 1, 2, ...).

Bound state | A state is called bound state if its position probability density at infinite tends to zero for all the time. Roughly speaking, we can expect to find the particle(s) in a finite size region with certain probability.

Bra–ket notation | The bra–ket notation is a way to represent the states and operators of a system by angle brackets and vertical bars, for example, |α> and |α><β|.

Collapse | "Collapse" means the sudden process which the state of the system will "suddenly" change to an eigenstate of the observable during measurement.

commutator | The commutator of two operators elements **a** and **b** is defined by **[a,b]=ab-ba**. The commutator is zero if and only if **a** and **b** commute.

commute | The commutator of two operators elements **a** and **b** is defined by **[a,b]=ab-ba**. The commutator is zero if and only if **a** and **b** commute.

Correspondence principle | For every observable property of a system there is a corresponding quantum mechanical operator.

cyclic boundary condition | A boundary condition associated with regularly repeating intervals. For quantum rigid rotors, this implied the wavefunction must equal itself upon a full rotation, i.e., $\psi(0^o)=\psi(360^o)$.

Degeneracy | If the energy of different states (wavefunctions that are not scalar multiple of each other) are the same, the states are called **degenerate**.

Degenerate energy level | If the energy of different state (wave functions which are not scalar multiple of each other) is the same, the energy level is called degenerate. There is no degeneracy in 1D system.

Density matrix | Physically, the density matrix is a way to represent pure states and mixed states. The density matrix of pure state whose ket is |α> is |α><α|.

Density operator | Physically, the density matrix is a way to represent pure states and mixed states. The density matrix of pure state whose ket is |α> is |α><α|.

dipole moment | The electric dipole moment is a measure of the separation of positive and negative electrical charges within a system and is a measure of the system's overall polarity.

Dirac notation | The bra–ket notation is a way to represent the states and operators of a system by angle brackets and vertical bars, for example, |α> and |α><β|.

Eigenstates | An eigenstate of an operator A is a vector satisfied the eigenvalue equation: A | a > = λ | a >, where λ is a scalar (the eigenvalue).

eigenvalue | Any value of λ that is is a solution to the eigenvalue problem (A·v=λ·v) is known as an eigenvalue of the matrix A.

eigenvalue equation | An eigenvalue problem is A·v=λ·v, where A is an n-by-n matrix, v is a non-zero n-by-1 vector and λ is a scalar (that can be real or complex).

eigenvector | Any value of v that is is a solution to the eigenvalue problem (A·v=λ·v) is known as an eigenvevctor of the matrix A.

Energy spectrum | The energy spectrum refers to the possible energy of a system.
For bound system (bound states), the energy spectrum is discrete; for unbound system (scattering states), the energy spectrum is continuous.

even function | A function is even if f(x)=f(-x)

Expectation value | The expectation value is the probabilistic expected value of the result (measurement) of an experiment. It can be thought of as an average of all the possible outcomes of a measurement as weighted by their likelihood, and as such it is not the most probable value of a measurement; indeed the expectation value may have zero probability of occurring

Fermions | Fermions are particles with half-integer spin (s = 1/2, 3/2, 5/2, ...).

Fine Structure Constant | 1/137 . The fine structure constant is a mathematical constant that is given as the ratio of the classical and quantum electromagnetic constants. It is also known as **Sommerfeld's constant.**

forbidden transition | A eigentstate to eigenstate transition with zero probability of being observed. This is determined by the relevant transition moment integral

g-factor | A dimensionless quantity that characterizes the magnetic moment and angular momentum of an atom, a particle or the nucleus. It is essentially a proportionality constant that relates the observed magnetic moment μ of a particle to its angular momentum quantum number and a unit of magnetic moment. (also known as spin gyromagnetic ratio)

gyromagnetic ratio | The ratio of its magnetic moment to its angular momentum, and it is often denoted by the symbol γ, gamma (also known as magnetogyric ratio)

Hamiltonian | The operator represents the total energy of the system.

Hermite polynomials | A family of orthogonal polynomials. In quantum mechanics, they results from solving the harmonic oscillator model.

Hermitian | A Hermitian matrix is a complex square matrix that is equal to its own conjugate transpose—that is, the element in the i-th row and j-th column is equal to the complex conjugate of the element in the j-th row and i-th column, for all indices i and j. aij=aji* . Hermitian matrices always have real eigenvalues. Operators connected to physical observable are Hermitian since observables must be real.

Hermitian operator | An operator satisfying $A = A^{\dagger}$.

Hilbert space | Given a system, the possible pure state can be represented as a vector in a Hilbert space. Each ray (vectors differ by phase and magnitude only) in the corresponding Hilbert space represent a state.

Identity operator | Operator that does not change the elements it operates on.

Indistinguishable particles | If a system shows measurable differences when one of its particles is replaced by another particle, these two particles are called distinguishable.

Ket | A wave function expressed in the form $|a\rangle$ is called a ket.

Lambshift | Relativistic correction of the difference in energy levels of the $^2S_{1/2}$ and $^2P_{1/2}$ hydrogen atom not predicted by the Dirac equation

Laplacian | The Laplacian is a differential operator that is given by the divergence of the gradient.

LCAO | This is is a simple method of quantum chemistry that yields a qualitative picture of the molecular orbitals in a molecule.

Legendre polynomials | A family of complete and orthogonal polynomials with numerous applications. In quantum mechanics, they results from solving the rigid rotor model.

Linear combination of atomic orbitals | This is is a simple method of quantum chemistry that yields a qualitative picture of the molecular orbitals in a molecule.

Maclaurin series | The Maclaurin series is an expansion of a function in an infinite sum of polynomial terms that are expressed in terms of the function's derivatives at **zero**.

magnetogyric ratio | The ratio of its magnetic moment to its angular momentum, and it is often denoted by the symbol γ, gamma (also known as magnetogyric ratio

Mixed state | A mixed state is a statistical ensemble of pure state.

molecular orbitals | A molecular orbital is a mathematical function describing the location and wave-like behavior of a single electron in a molecule. This function can be used to calculate chemical and physical properties such as the probability of finding an electron in any specific region. The LCAO approximation is often used to approximate molecular orbitals as a series of atomic orbitals

node | Location where the quantum mechanical wavefunction is zero and therefore, with no probability amplitude.

Normalized wave function | A wave function |a > is said to be normalized if < a | a> = 1.

Observable | Mathematically, it is represented by a Hermitian operator.

observer effect | When an observed system is disturbed by the act of observation. This is often the result of instruments that, by necessity, alter the state of what they measure in some manner.

odd function | A function is odd if -f(x)=f(-x)

operator | A mathematical entity that transforms one function into another [Richard Fitzpatrick]

orbital angular momentum | The classical definition of angular momentum is L = r × p. The quantum-mechanical counterparts of these objects share the same relationship where r is the quantum position operator, p is the quantum momentum operator, × is cross product, and L is the orbital angular momentum operator. L (just like p and r) is a vector operator whose components operators are L_x, L_y, L_z, which are the projection of L on the x, y, and z axis, respectively

overtone | A band that occurs in a vibrational spectrum of molecule that is associated with the transition from the ground state (v=0) to the second excited state (v=2).

Pauli exclusion principle | The principle that two or more identical fermions (e.g., electrons) cannot occupy the same quantum state within the same quantum system simultaneously. An alternative formulation is that no two fermions can have the same set of quantum numbers in a system

Pure state | A state which can be represented as a wave function / ket in Hilbert space / solution of Schrödinger equation is called pure state. See "mixed state".

Quantum numbers | A way of representing a state by several numbers

Radial distribution function | The square of the radial distribution function describes the probability of finding an a electron a given distance from the nucleus. This is related to the radial probability density by adding a factor of $4\pi r^2$ (the volumen element of a sphere). The radial distribution functions depend on both n and l.

radial node | A radial node will occur where the radial part of the electronic wavefunction equals zero.

radial probability density | The probability density for the electron to be at a point located the distance r from the nucleus. The radial radial probability density depend on both n and l.

reduced mass | The "effective" inertial mass appearing in the two-body problems. It is a quantity which allows two-body problems to be solved as if they were one-body problems.

rotational constant | A constant commonly used to describe molecular free rotation that depends on the distribution of mass within the molecule (i.e, moment of inertia, I) and other constants: $B=h/(8\pi^2cI)$

selection rule | Selection rules describes when the probability of transitioning from one level to another cannot be zero. They explicitly come from evaluating the relevant transition moment integral

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spherical harmonics | Spherical harmonics are functions of the spherical polar angles θ and φ and appear as eigenfunctions of (squared) orbital angular momentum. They form an orthogonal and complete set. Any harmonic is a function that satisfies Laplace's differential equation.

spin | Spin is a quantized property of all particles, both matter and force, in the Universe. Matter particles have half-integer spin (1/2, 3/2,…) and force particles integer spin (0, 1, 2,…). Spin is intrinsic angular momentum possessed by the particles. The spin of a particle is sort of analogous to that of a spinning top, except that the particle can only spin at one speed, can't stop or even slow down, and is infinitesimally small. It is important to note that in no way are the particles actually spinning. [CC-BY-SA]

spin gyromagnetic ratio | A dimensionless quantity that characterizes the magnetic moment and angular momentum of an atom, a particle or the nucleus. It is essentially a proportionality constant that relates the observed magnetic moment μ of a particle to its angular momentum quantum number and a unit of magnetic moment. (also known as g-factor)

square-integrable | A square-integrable function is a real- or complex-valued measurable function for which the integral of the **square** of the absolute value is finite.

State vector | synonymous to "wave function".

Stationary state | A stationary state of a bound system is an eigenstate of Hamiltonian operator. Classically, it corresponds to standing wave.

stationary states | This is a quantum state with all observables independent of time. It is an eigenvector of the Hamiltonian.

Taylor series | The Taylor series is an expansion of a function in an infinite sum of polynomial terms that are expressed in terms of the function's derivatives at a single point.

Time-Independent Schrödinger Equation | A modification of the Time-Dependent Schrödinger equation as an eigenvalue problem. The solutions are energy eigenstate of the system.

transition moment integral | The integral representing the probability for a transition between an initial eigenstate and a final eignestate by the absorption or emission of photon(s)

uncertainty principle | The uncertainty principle (put forward by Werner Heisenberg) states that there will always be an intrinsic uncertainty in determining both a particle's position and momentum (i.e., you cannot know both exactly at the same time). This has nothing to do with science's ability to detect the properties of momentum and position. [CC-BY-SA]

wavenumber | The wavenumber is a unit of frequency that is equal to the frequency (in Hertz) divided by the speed of light. This is typically in unit of cm^{-1}. Since wavenumbers are proportional to frequency, and to photon energy (by E=hν), it is also a unit of energy.

zero point motion | Fluctuation in the position of an object necessitated by having zero point energy. This is a consequence of the Heisenberg uncertainty principle.

Zero-point energy | Zero-point energy (ZPE) is the lowest possible energy that a quantum mechanical system may have.