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How to use schrodinger wave equation

Description of a quantum-mechanical system For a more general introduction to the topic, see Introduction to quantum mechanics. Part of a series of articles aboutQuantum mechanics i ℏ ∂ ∂ t | ψ (t) ⟩ = H ^ | ψ (t) ⟩ {\displaystyle i\hbar {\frac {\partial }{\partial t}}|\psi (t)\rangle ={\hat {H}}|\psi (t)\rangle } Schrödinger equation Introduction Glossary History Background Classical mechanics Old quantum theory Bra–ket notation Hamiltonian Interference Fundamentals Complementarity Decoherence Entanglement Energy level Measurement Nonlocality Quantum number State Superposition Symmetry Tunnelling Uncertainty Wave function Collapse Experiments Bell's inequality Davisson–Germer Double-slit Elitzur–Vaidman Franck–Hertz Leggett–Garg inequality Mach–Zehnder Popper Quantum eraser Delayed-choice Schrödinger's cat Stern–Gerlach Wheeler's delayed-choice Formulations Overview Heisenberg Interaction Matrix Phase-space Schrödinger Sum-over-histories (path integral) Equations Dirac Klein–Gordon Pauli Rydberg Schrödinger Interpretations Overview Bayesian Consistent histories Copenhagen de Broglie–Bohm Ensemble Hidden-variable Local Many-worlds Objective collapse Quantum logic Relational Transactional Advanced topics Relativistic quantum mechanics Quantum field theory Quantum information science Quantum computing Quantum chaos Density matrix Scattering theory Quantum statistical mechanics Quantum machine learning Scientists Aharonov Bell Bethe Blackett Bloch Bohm Bohr Born Bose de Broglie Compton Dirac Davisson Debye Ehrenfest Einstein Everett Fock Fermi Feynman Glauber Gutzwiller Heisenberg Hilbert Jordan Kramers Pauli Lamb Landau Laue Moseley Millikan Onnes Planck Rabi Raman Rydberg Schrödinger Simmons Sommerfeld von Neumann Weyl Wien Wigner Zeeman Zeilinger vte Modern physics H ^ | ψ n (t) ⟩ = i ℏ ∂ ∂ t | ψ n (t) ⟩ {\displaystyle {\hat {H}}|\psi _{n}(t)\rangle =i\hbar {\frac {\partial }{\partial t}}|\psi _{n}(t)\rangle } 1 c 2 ∂ 2 ϕ n ∂ t 2 − ∇ 2 ϕ n + (m c ℏ) 2 ϕ n = 0 {\displaystyle {\frac {1}{{c}^{2}}}{\frac {{\partial }^{2}{\phi }_{n}}{{\partial t}^{2}}}-{{abla }^{2}{\phi }_{n}}+{\left({\frac {mc}{\hbar }}\right)}^{2}{\phi }_{n}=0} Manifold dynamics: Schrödinger and Klein–Gordon equations FoundersMax Planck · Albert Einstein · Niels Bohr · Max Born · Werner Heisenberg · Erwin Schrödinger · Pascual Jordan · Wolfgang Pauli · Paul Dirac · Ernest Rutherford · Louis de Broglie · Satyendra Nath Bose ConceptsTopology · Space · Time · Energy · Matter · Work Randomness · Information · Entropy · Mind Light · Particle · Wave BranchesApplied · Experimental · Theoretical Mathematical · Philosophy of physics Quantum mechanics (Quantum field theory · Quantum information · Quantum computation) Electromagnetism · Weak interaction · Electroweak interaction Strong interaction Atomic · Particle · Nuclear Atomic, molecular, and optical Condensed matter · Statistical Complex systems · Non-linear dynamics · Biophysics Neurophysics Plasma physics Special relativity · General relativity Astrophysics · Cosmology Theories of gravitation Quantum gravity · Theory of everything ScientistsWitten · Röntgen · Becquerel · Lorentz · Planck · Curie · Wien · Skłodowska-Curie · Sommerfeld · Rutherford · Soddy · Onnes · Einstein · Wilczek · Born · Weyl · Bohr · Kramers · Schrödinger · de Broglie · Laue · Bose · Compton · Pauli · Walton · Fermi · van der Waals · Heisenberg · Dyson · Zeeman · Moseley · Hilbert · Gödel · Jordan · Dirac · Wigner · Hawking · P. W. Anderson · Lemaître · Thomson · Poincaré · Wheeler · Penrose · Millikan · Nambu · von Neumann · Higgs · Hahn · Feynman · Yang · Lee · Lenard · Salam · 't Hooft · Veltman · Bell · Gell-Mann · J. J. Thomson · Raman · Bragg · Bardeen · Shockley · Chadwick · Lawrence · Zeilinger · Goudsmit · Uhlenbeck Categories Modern physics vte Schrödinger's equation inscribed on the gravestone of Annemarie and Erwin Schrödinger. (Newton's dot notation for the time derivative is used.) The Schrödinger equation is a linear partial differential equation that governs the wave function of a quantum-mechanical system.[1]:1–2 It is a key result in quantum mechanics, and its discovery was a significant landmark in the development of the subject. The equation is named after Erwin Schrödinger, who postulated the equation in 1925, and published it in 1926, forming the basis for the work that resulted in his Nobel Prize in Physics in 1933.[2][3] Conceptually, the Schrödinger equation is the quantum counterpart of Newton's second law in classical mechanics. Given a set of known initial conditions, Newton's second law makes a mathematical prediction as to what path a given physical system will take over time. The Schrödinger equation gives the evolution over time of a wave function, the quantum-mechanical characterization of an isolated physical system. The equation can be derived from the fact that the time-evolution operator must be unitary, and must therefore be generated by the exponential of a self-adjoint operator, which is the quantum Hamiltonian. The Schrödinger equation is not the only way to study quantum mechanical systems and make predictions. The other formulations of quantum mechanics include matrix mechanics, introduced by Werner Heisenberg, and the path integral formulation, developed chiefly by Richard Feynman. Paul Dirac incorporated matrix mechanics and the Schrödinger equation into a single formulation. When these approaches are compared, the use of the Schrödinger equation is sometimes called "wave mechanics". Definition Preliminaries Complex plot of a wave function that satisfies the nonrelativistic Schrödinger equation with V = 0. In other words, this corresponds to a particle traveling freely through empty space. Introductory courses on physics or chemistry typically introduce the Schrödinger equation in a way that can be appreciated knowing only the concepts and notations of basic calculus, particularly derivatives with respect to space and time. A special case of the Schrödinger equation that admits a statement in those terms is the position-space Schrödinger equation for a single nonrelativistic particle in one dimension: i ℏ ∂ ∂ t Ψ (x , t) = [− ℏ 2 2 m ∂ 2 ∂ x 2 + V (x , t)] Ψ (x , t) . {\displaystyle i\hbar {\frac {\partial }{\partial t}}\Psi (x,t)=\left[-{\frac {\hbar ^{2}}{2m}}{\frac {\partial ^{2}}{\partial x^{2}}}+V(x,t)\right]\Psi (x,t).} Here, Ψ (x , t) {\displaystyle \Psi (x,t)} is a wave function, a function that assigns a complex number to each point x {\displaystyle x} at each time t {\displaystyle t} . The parameter m {\displaystyle m} is the mass of the particle, and V (x , t) {\displaystyle V(x,t)} is the potential that represents the environment in which the particle exists. The constant i {\displaystyle i} is the imaginary unit, and ℏ {\displaystyle \hbar } is the reduced Planck constant, which has units of action (energy multiplied by time). Broadening beyond this simple case, the mathematical formulation of quantum mechanics developed by Paul Dirac,[4] David Hilbert,[5] John von Neumann,[6] and Hermann Weyl[7] defines the state of a quantum mechanical system to be a vector | ψ ⟩ {\displaystyle |\psi \rangle } belonging to a (separable) Hilbert space H {\displaystyle {\mathcal {H}}} . This vector is postulated to be normalized under the Hilbert's space inner product, that is, in Dirac notation it obeys ⟨ ψ | ψ ⟩ = 1 {\displaystyle \langle \psi |\psi \rangle =1} . The exact nature of this Hilbert space is dependent on the system – for example, for describing position and momentum the Hilbert space is the space of complex square-integrable functions L 2 (C) {\displaystyle L^{2}(\mathbb {C})} , while the Hilbert space for the spin of a single proton is simply the space of two-dimensional complex vectors C 2 {\displaystyle \mathbb {C} ^{2}} with the usual inner product. Physical quantities of interest — position, momentum, energy, spin — are represented by "observables", which are Hermitian (more precisely, self-adjoint) linear operators acting on the Hilbert space. A wave function can be an eigenvector of an observable, in which case it is called an eigenstate, and the associated eigenvalue corresponds to the value of the observable in that eigenstate. More generally, a quantum state will be a linear combination of the eigenstates, known as a quantum superposition. When an observable is measured, the result will be one of its eigenvalues with probability given by the Born rule: in the simplest case the eigenvalue λ {\displaystyle \lambda } is non-degenerate and the probability is given by | ⟨ λ | ψ ⟩ | 2 {\displaystyle |\langle \lambda |\psi \rangle |^{2}} , where | λ ⟩ {\displaystyle |\lambda \rangle } is its associated eigenvector. More generally, the eigenvalue is degenerate and the probability is given by ⟨ ψ | P λ | ψ ⟩ {\displaystyle \langle \psi |P_{\lambda }|\psi \rangle } , where P λ {\displaystyle P_{\lambda }} is the projector onto its associated eigenspace.[note 1] A momentum eigenstate would be a perfectly monochromatic wave of infinite extent, which is not square-integrable. Likewise, a position eigenstate would be a Dirac delta distribution, not square-integrable and technically not a function at all. Consequently, neither can belong to the particle's Hilbert space. Physicists sometimes introduce fictitious "bases" for a Hilbert space comprising elements outside that space. These are invented for calculational convenience and do not represent physical states.[8]:100–105 Thus, a position-space wave function Ψ (x , t) {\displaystyle \Psi (x,t)} as used above can be written as the inner product of a time-dependent state vector | Ψ (t) ⟩ {\displaystyle |\Psi (t)\rangle } with unphysical but convenient "position eigenstates" | x ⟩ {\displaystyle |x\rangle } : Ψ (x , t) = ⟨ x | Ψ (t) ⟩ . {\displaystyle \Psi (x,t)=\langle x|\Psi (t)\rangle .} Time-dependent equation The form of the Schrödinger equation depends on the physical situation. The most general form is the time-dependent Schrödinger equation, which gives a description of a system evolving with time:[9]:143 Time-dependent Schrödinger equation (general) i ℏ d d t | Ψ (t) ⟩ = H ^ | Ψ (t) ⟩ {\displaystyle i\hbar {\frac {d}{dt}}\vert \Psi (t)\rangle ={\hat {H}}\vert \Psi (t)\rangle } where t {\displaystyle t} is time, | Ψ (t) ⟩ {\displaystyle \vert \Psi (t)\rangle } is the state vector of the quantum system (Ψ {\displaystyle \Psi } being the Greek letter psi), and H ^ {\displaystyle {\hat {H}}} is an observable, the Hamiltonian operator. Each of these three rows is a wave function which satisfies the time-dependent Schrödinger equation for a harmonic oscillator. Left: The real part (blue) and imaginary part (red) of the wave function. Right: The probability distribution of finding the particle with this wave function at a given position. The top two rows are examples of stationary states, which correspond to standing waves. The bottom row is an example of a state which is not a stationary state. The right column illustrates why stationary states are called "stationary". The term "Schrödinger equation" can refer to both the general equation, or the specific nonrelativistic version. The general equation is indeed quite general, used throughout quantum mechanics, for everything from the Dirac equation to quantum field theory, by plugging in diverse expressions for the Hamiltonian. The specific nonrelativistic version is an approximation that yields accurate results in many situations, but only to a certain extent (see relativistic quantum mechanics and relativistic quantum field theory). To apply the Schrödinger equation, write down the Hamiltonian for the system, accounting for the kinetic and potential energies of the particles constituting the system, then insert it into the Schrödinger equation. The resulting partial differential equation is solved for the wave function, which contains information about the system. In practice, the square of the absolute value of the wave function at each point is taken to define a probability density function. For example, given a wave function in position space Ψ (x , t) {\displaystyle \Psi (x,t)} as above, we have Pr (x , t) = | Ψ (x , t) | 2 . {\displaystyle \Pr(x,t)=|\Psi (x,t)|^{2}.} Time-independent equation The time-dependent Schrödinger equation described above predicts that wave functions can form standing waves, called stationary states. These states are particularly important as their individual study later simplifies the task of solving the time-dependent Schrödinger equation for any state. Stationary states can also be described by a simpler form of the Schrödinger equation, the time-independent Schrödinger equation. Time-independent Schrödinger equation (general) H ^ | Ψ ⟩ = E | Ψ ⟩ {\displaystyle \operatorname {\hat {H}} |\Psi \rangle =E|\Psi \rangle } where E {\displaystyle E} is the energy of the system. This is only used when the Hamiltonian itself is not dependent on time explicitly. However, even in this case the total wave function is dependent on time as explained in the section on linearity below. In the language of linear algebra, this equation is an eigenvalue equation. Therefore, the wave function is an eigenfunction of the Hamiltonian operator with corresponding eigenvalue(s) E {\displaystyle E} . Properties Linearity The Schrödinger equation is a linear differential equation, meaning that if two state vectors | ψ 1 ⟩ {\displaystyle |\psi _{1}\rangle } and | ψ 2 ⟩ {\displaystyle |\psi _{2}\rangle } are solutions, then so is any linear combination | ψ ⟩ = a | ψ 1 ⟩ + b | ψ 2 ⟩ {\displaystyle |\psi \rangle =a|\psi _{1}\rangle +b|\psi _{2}\rangle } of the two where a and b are any complex numbers.[10]:25 Moreover, the sum can be extended for any number of state vectors. This property allows superpositions of quantum states to be solutions of the Schrödinger equation. Even more generally, it holds that a general solution to the Schrödinger equation can be found by taking a weighted sum over a basis of states. A choice often employed is the basis of energy eigenstates, which are solutions of the time-independent Schrödinger equation. In this basis, a time-dependent state vector | Ψ (t) ⟩ {\displaystyle |\Psi (t)\rangle } can be written as the linear combination | Ψ (t) ⟩ = ∑ n A n e − i E n t / ℏ | ψ E n ⟩ , {\displaystyle |\Psi (t)\rangle =\sum _{n}A_{n}e^{{-iE_{n}t}/\hbar }|\psi _{E_{n}}\rangle ,} where A n {\displaystyle A_{n}} are complex numbers and the vectors | ψ E n ⟩ {\displaystyle |\psi _{E_{n}}\rangle } are solutions of the time-independent equation H ^ | ψ E n ⟩ = E n | ψ E n ⟩ {\displaystyle {\hat {H}}|\psi _{E_{n}}\rangle =E_{n}|\psi _{E_{n}}\rangle } . Unitarity Further information: Wigner's theorem Holding the Hamiltonian H ^ {\displaystyle {\hat {H}}} constant, the Schrödinger equation has the solution[9] | Ψ (t) ⟩ = e − i H ^ t / ℏ | Ψ (0) ⟩ . {\displaystyle |\Psi (t)\rangle =e^{-i{\hat {H}}t/\hbar }|\Psi (0)\rangle .} The operator U ^ (t) = e − i H ^ t / ℏ {\displaystyle {\hat {U}}(t)=e^{-i{\hat {H}}t/\hbar }} is known as the time-evolution operator, and it is unitary: it preserves the inner product between vectors in the Hilbert space.[10] Unitarity is a general feature of time evolution under the Schrödinger equation. If the initial state is | Ψ (0) ⟩ {\displaystyle |\Psi (0)\rangle } , then the state at a later time t {\displaystyle t} will be given by | Ψ (t) ⟩ = U ^ (t) | Ψ (0) ⟩ {\displaystyle |\Psi (t)\rangle ={\hat {U}}(t)|\Psi (0)\rangle } for some unitary operator U ^ (t) {\displaystyle {\hat {U}}(t)} . Conversely, suppose that U ^ (t) {\displaystyle {\hat {U}}(t)} is a continuous family of unitary operators parameterized by t {\displaystyle t} . Without loss of generality,[11] the parameterization can be chosen so that U ^ (0) {\displaystyle {\hat {U}}(0)} is the identity operator and that U ^ (t / N) N = U ^ (t) {\displaystyle {\hat {U}}(t/N)^{N}={\hat {U}}(t)} for any N > 0 {\displaystyle N>0} . Then U ^ (t) {\displaystyle {\hat {U}}(t)} depends upon the parameter t {\displaystyle t} in such a way that U ^ (t) = e − i G ^ t {\displaystyle {\hat {U}}(t)=e^{-i{\hat {G}}t}} for some self-adjoint operator G ^ {\displaystyle {\hat {G}}} , called the generator of the family U ^ (t) {\displaystyle {\hat {U}}(t)} . A Hamiltonian is just such a generator (up to the factor of Planck's constant that would be set to 1 in natural units). To see that the generator is Hermitian, note that with U ^ (δ t) ≈ U ^ (0) − i G ^ δ t {\displaystyle {\hat {U}}(\delta t)\approx {\hat {U}}(0)-i{\hat {G}}\delta t} , we have U ^ (δ t) † U ^ (δ t) ≈ (U ^ (0) † + i G ^ † δ t) (U ^ (0) − i G ^ δ t) = I + i δ t (G ^ † − G ^) + O (δ t 2) , {\displaystyle {\hat {U}}(\delta t)^{\dagger }{\hat {U}}(\delta t)\approx ({\hat {U}}(0)^{\dagger }+i{\hat {G}}^{\dagger }\delta t)({\hat {U}}(0)-i{\hat {G}}\delta t)=I+i\delta t({\hat {G}}^{\dagger }-{\hat {G}})+O(\delta t^{2}),} so U ^ (t) {\displaystyle {\hat {U}}(t)} is unitary only if, to first order, its derivative is Hermitian.[12] Changes of basis The Schrödinger equation is often presented using quantities varying as functions of position, but as a vector-operator equation it has a valid representation in any arbitrary complete basis of kets in Hilbert space. As mentioned above, "bases" that lie outside the physical Hilbert space are also employed for calculational purposes. This is illustrated by the position-space and momentum-space Schrödinger equations for a nonrelativistic, spinless particle.[8]:182 The Hilbert space for such a particle is the space of complex square-integrable functions on three-dimensional Euclidean space, and its Hamiltonian is the sum of a kinetic-energy term that is quadratic in the momentum operator and a potential-energy term: i ℏ d d t | Ψ (t) ⟩ = (1 2 m p ^ 2 + V ^) | Ψ (t) ⟩ . {\displaystyle i\hbar {\frac {d}{dt}}|\Psi (t)\rangle =\left({\frac {1}{2m}}{\hat {p}}^{2}+{\hat {V}}\right)|\Psi (t)\rangle .} Writing r {\displaystyle \mathbf {r} } for a three-dimensional position vector and p {\displaystyle \mathbf {p} } for a three-dimensional momentum vector, the position-space Schrödinger equation is i ℏ ∂ ∂ t Ψ (r , t) = − ℏ 2 2 m ∇ 2 Ψ (r , t) + V (r) Ψ (r , t) . {\displaystyle i\hbar {\frac {\partial }{\partial t}}\Psi (\mathbf {r} ,t)=-{\frac {\hbar ^{2}}{2m}}abla ^{2}\Psi (\mathbf {r} ,t)+V(\mathbf {r})\Psi (\mathbf {r} ,t).} The momentum-space counterpart involves the Fourier transforms of the wave function and the potential: i ℏ ∂ ∂ t Ψ ~ (p , t) = p 2 2 m Ψ ~ (p , t) + (2 π ℏ) − 3 / 2 ∫ d 3 p ′ V ~ (p − p ′) Ψ ~ (p ′ , t) . {\displaystyle i\hbar {\frac {\partial }{\partial t}}\tilde {\Psi }(\mathbf {p} ,t)={\frac {\mathbf {p} ^{2}}{2m}}\tilde {\Psi }(\mathbf {p} ,t)+(2\pi \hbar)^{-3/2}\int d^{3}\mathbf {p} '\,{\tilde {V}}(\mathbf {p} -\mathbf {p} ')\tilde {\Psi }(\mathbf {p} ',t).} The functions Ψ (r , t) {\displaystyle \Psi (\mathbf {r} ,t)} and Ψ ~ (p , t) {\displaystyle {\tilde {\Psi }}(\mathbf {p} ,t)} are derived from | Ψ (t) ⟩ {\displaystyle |\Psi (t)\rangle } by Ψ (r , t) = ⟨ r | Ψ (t) ⟩ , {\displaystyle \Psi (\mathbf {r} ,t)=\langle \mathbf {r} |\Psi (t)\rangle ,} Ψ ~ (p , t) = ⟨ p | Ψ (t) ⟩ , {\displaystyle {\tilde {\Psi }}(\mathbf {p} ,t)=\langle \mathbf {p} |\Psi (t)\rangle ,} where | r ⟩ {\displaystyle |\mathbf {r} \rangle } and | p ⟩ {\displaystyle |\mathbf {p} \rangle } do not belong to the Hilbert space itself, but have well-defined inner products with all elements of that space. When restricted from three dimensions to one, the position-space equation is just the first form of the Schrödinger equation given above. The relation between position and momentum in quantum mechanics can be appreciated in a single dimension. In canonical quantization, the classical variables x {\displaystyle x} and p {\displaystyle p} are promoted to self-adjoint operators x ^ {\displaystyle {\hat {x}}} and p ^ {\displaystyle {\hat {p}}} that satisfy the canonical commutation relation [x ^ , p ^] = i ℏ . {\displaystyle [{\hat {x}},{\hat {p}}]=i\hbar .} This implies that[8]:190 ⟨ x | p ^ | Ψ ⟩ = − i ℏ d d x Ψ (x) , {\displaystyle \langle x|{\hat {p}}|\Psi \rangle =-i\hbar {\frac {d}{dx}}\Psi (x),} so the action of the momentum operator p ^ {\displaystyle {\hat {p}}} in the position-space representation is − i ℏ d d x {\textstyle -i\hbar {\frac {d}{dx}}} . Thus, p ^ 2 {\displaystyle {\hat {p}}^{2}} becomes a second derivative, and in three dimensions, the second derivative becomes the Laplacian ∇ 2 {\displaystyle abla ^{2}} . The canonical commutation relation also implies that the position and momentum operators are Fourier conjugates of each other. Consequently, functions originally defined in terms of their position dependence can be converted to functions of momentum using the Fourier transform. In solid-state physics, the Schrödinger equation is often written for functions of momentum, as Bloch's theorem ensures the periodic crystal lattice potential couples Ψ ~ (p) {\displaystyle {\tilde {\Psi }}(p)} with Ψ ~ (p + K) {\displaystyle {\tilde {\Psi }}(p+K)} for only discrete reciprocal lattice vectors K {\displaystyle K} . This makes it convenient to solve the momentum-space Schrödinger equation at each point in the Brillouin zone independently of the other points in the Brillouin zone. Probability current Main articles: Probability current and Continuity equation The Schrödinger equation is consistent with local probability conservation.[8]:238 Multiplying the Schrödinger equation on the right by the complex conjugate wave function, and multiplying the wave function to the left of the complex conjugate of the Schrödinger equation, and subtracting, gives the continuity equation for probability: ∂ ∂ t ρ (r , t) + ∇ ⋅ j = 0 , {\displaystyle {\frac {\partial }{\partial t}}\rho \left(\mathbf {r} ,\right)+abla \cdot \mathbf {j} =0,} where ρ = | Ψ | 2 = Ψ ∗ (r , t) Ψ (r , t) {\displaystyle \rho =|\Psi |^{2}=\Psi ^{*}(\mathbf {r} ,t)\Psi (\mathbf {r} ,t)} is the probability density (probability per unit volume, * denotes complex conjugate), and j = 1 2 m (Ψ ∗ p ^ Ψ − Ψ p ^ Ψ ∗) {\displaystyle \mathbf {j} ={\frac {1}{2m}}\left(\Psi ^{*}{\hat {\mathbf {p} }}\Psi -\Psi {\hat {\mathbf {p} }}\Psi ^{*}\right)} is the probability current (flow per unit area). Separation of variables If the Hamiltonian is not an explicit function of time, the equation is separable into a product of spatial and temporal parts.[13] Solving the equation by separation of variables means seeking a solution of the form Ψ (r , t) = ψ (r) τ (t) , {\displaystyle \Psi (\mathbf {r} ,t)=\psi (\mathbf {r})\tau (t),} where ψ (r) {\displaystyle \psi (\mathbf {r})} is a function of all the spatial coordinate(s) of the particle(s) constituting the system only, and τ (t) {\displaystyle \tau (t)} is a function of time only. Substituting this expression for Ψ {\displaystyle \Psi } into the Schrödinger equation yields Ψ (r , t) = ψ (r) e − i E t / ℏ . {\displaystyle \Psi (\mathbf {r} ,t)=\psi (\mathbf {r})e^{-i{Et/\hbar }}.} A solution of this type is called stationary, since the only time dependence is a phase factor that cancels when the probability density is calculated via the Born rule.[9]:143ff This generalizes to any number of particles in any number of dimensions (in a time-independent potential): the standing wave solutions of the time-dependent equation are the states with definite energy, instead of a probability distribution of different energies. In physics, these standing waves are called "stationary states" or "energy eigenstates"; in chemistry they are called "atomic orbitals" or "molecular orbitals". Superpositions of energy eigenstates change their properties according to the relative phases between the energy levels. The energy eigenstates form a basis: any wave function may be written as a sum over the discrete energy states or an integral over continuous energy states, or more generally as an integral over a measure. This is the spectral theorem in mathematics, and in a finite-dimensional state space it is just a statement of the completeness of the eigenvectors of a Hermitian matrix. Separation of variables can also be a useful method for the time-independent Schrödinger equation. For example, depending on the symmetry of the problem, the Cartesian axes might be separated, ψ (r) = ψ x (x) ψ y (y) ψ z (z) , {\displaystyle \psi (\mathbf {r})=\psi _{x}(x)\psi _{y}(y)\psi _{z}(z),} or radial and angular coordinates might be separated: ψ (r) = ψ r (r) ψ θ (θ) ψ ϕ (ϕ) . {\displaystyle \psi (\mathbf {r})=\psi _{r}(r)\psi _{\theta }(\theta)\psi _{\phi }(\phi).} Examples See also: List of quantum-mechanical systems with analytical solutions Particle in a box 1-dimensional potential energy box (or infinite potential well) Main article: Particle in a box The particle in a one-dimensional potential energy box is the most mathematically simple example where restraints lead to the quantization of energy levels. The box is defined as having zero potential energy inside a certain region and infinite potential energy outside.[8]:77–78 For the one-dimensional case in the x {\displaystyle x} direction, the time-independent Schrödinger equation may be written − ℏ 2 2 m d 2 ψ d x 2 = E ψ . {\displaystyle -{\frac {\hbar ^{2}}{2m}}{\frac {d^{2}\psi }{dx^{2}}}=E\psi .} With the differential operator defined by p ^ x = − i ℏ d d x {\displaystyle {\hat {p}}_{x}=-i\hbar {\frac {d}{dx}}} the previous equation is evocative of the classic kinetic energy analogue, 1 2 m p ^ x 2 = E , {\displaystyle {\frac {1}{2m}}{\hat {p}}_{x}^{2}=E,} with state ψ {\displaystyle \psi } in this case having energy E {\displaystyle E} coincident with the kinetic energy of the particle. The general solutions of the Schrödinger equation for the particle in a box are ψ (x) = A e i k x + B e − i k x E = ℏ 2 k 2 2 m {\displaystyle \psi (x)=Ae^{ikx}+Be^{-ikx}\qquad \qquad E={\frac {\hbar ^{2}k^{2}}{2m}}} or, from Euler's formula, ψ (x) = C sin ⁡ (k x) + D cos ⁡ (k x) . {\displaystyle \psi (x)=C\sin(kx)+D\cos(kx).} The infinite potential walls of the box determine the values of C , D , {\displaystyle C,D,} and k {\displaystyle k} at x = 0 {\displaystyle x=0} and x = L {\displaystyle x=L} where ψ {\displaystyle \psi } must be zero. Thus, at x = 0 {\displaystyle x=0} , ψ (0) = 0 = C sin ⁡ (0) + D cos ⁡ (0) = D {\displaystyle \psi (0)=0=C\sin(0)+D\cos(0)=D} and D = 0 {\displaystyle D=0} . At x = L {\displaystyle x=L} , ψ (L) = 0 = C sin ⁡ (k L) , {\displaystyle \psi (L)=0=C\sin(kL),} in which C {\displaystyle C} cannot be zero as this would conflict with the postulate that ψ {\displaystyle \psi } has norm 1. Therefore, since sin ⁡ (k L) = 0 {\displaystyle \sin(kL)=0} , k L {\displaystyle kL} must be an integer multiple of π {\displaystyle \pi } , k = n π L n = 1 , 2 , 3 , … . {\displaystyle k={\frac {n\pi }{L}}\qquad \qquad n=1,2,3,\ldots .} This constraint on k {\displaystyle k} implies a constraint on the energy levels, yielding E n = ℏ 2 π 2 n 2 2 m L 2 = n 2 h 2 8 m L 2 . {\displaystyle E_{n}={\frac {\hbar ^{2}\pi ^{2}n^{2}}{2mL^{2}}}={\frac {n^{2}h^{2}}{8mL^{2}}}.} A finite potential well is the generalization of the infinite potential well problem to potential wells having finite depth. The finite potential well problem is mathematically more complicated than the infinite particle-in-a-box problem as the wave function is not pinned to zero at the walls of the well. Instead, the wave function must satisfy more complicated mathematical boundary conditions as it is nonzero in regions outside the well. Another related problem is that of the rectangular potential barrier, which furnishes a model for the quantum tunneling effect that plays an important role in the performance of modern technologies such as flash memory and scanning tunneling microscopy. Harmonic oscillator A harmonic oscillator in classical mechanics (A–B) and quantum mechanics (C–H). In (A–B), a ball, attached to a spring, oscillates back and forth. (C–H) are six solutions to the Schrödinger Equation for this situation. The horizontal axis is real part (blue) or imaginary part (red) of the wave function. Stationary states, or energy eigenstates, which are solutions to the time-independent Schrödinger equation, are shown in C, D, E, F, but not G or H. Main article: Quantum harmonic oscillator The Schrödinger equation for this situation is E ψ = − ℏ 2 2 m d 2 d x 2 ψ + 1 2 m ω 2 x 2 ψ , {\displaystyle E\psi =-{\frac {\hbar ^{2}}{2m}}{\frac {d^{2}}{dx^{2}}}\psi +{\frac {1}{2}}m\omega ^{2}x^{2}\psi ,} where x {\displaystyle x} is the displacement and ω {\displaystyle \omega } the angular frequency. Furthermore, it can be used to describe approximately a wide variety of other systems, including vibrating atoms, molecules,[14] and atoms or ions in lattices,[15] and approximating other potentials near equilibrium points. It is also the basis of perturbation methods in quantum mechanics. The solutions in position space are ψ n (x) = 1 2 n n ! ⋅ (m ω π ℏ) 1 / 4 ⋅ e − m ω x 2 2 ℏ ⋅ H n (m ω ℏ x) , {\displaystyle \psi _{n}(x)={\sqrt {\frac {1}{2^{n}\,n!}}}\ \left({\frac {m\omega }{\pi \hbar }}\right)^{1/4}\ e^{-{\frac {m\omega x^{2}}{2\hbar }}}\ \mathcal {H}}_{n}\left({\sqrt {\frac {m\omega }{\hbar }}}x\right),} where n ∈ { 0 , 1 , 2 , ... } {\displaystyle n\in \{0,1,2,\ldots \}} , and the functions H n {\displaystyle {\mathcal {H}}_{n}} are the Hermite polynomials of order n {\displaystyle n} . The solution set may be generated by ψ n (x) = 1 n ! ⋅ (m ω 2 ℏ) n (x − ℏ m ω d d x) n (m ω π ℏ) 1 4 e − m ω x 2 2 ℏ . {\displaystyle \psi _{n}(x)={\frac {1}{\sqrt {n!}}}\left({\sqrt {\frac {m\omega }{2\hbar }}}\right)^{n}\left(x-{\frac {\hbar }{m\omega }}{\frac {d}{dx}}\right)^{n}\left({\frac {m\omega }{\pi \hbar }}\right)^{\frac {1}{4}}e^{\frac {-m\omega x^{2}}{2\hbar }}.} The eigenvalues are E n = (n + 1 2) ℏ ω . {\displaystyle E_{n}=\left(n+{\frac {1}{2}}\right)\hbar \omega .} The case n = 0 {\displaystyle n=0} is called the ground state, its energy is called the zero-point energy, and the wave function is a Gaussian.[16] The harmonic oscillator, like the particle in a box, illustrates the generic feature of the Schrödinger equation that the energies of bound eigenstates are discretized.[8]:352 Hydrogen atom The Schrödinger equation for the hydrogen atom (or a hydrogen-like atom) is E ψ = − ℏ 2 2 μ ∇ 2 ψ − q 2 4 π ε 0 r ψ {\displaystyle E\psi =-{\frac {\hbar ^{2}}{2\mu }}abla ^{2}\psi -{\frac {q^{2}}{4\pi \varepsilon _{0}r}}\psi } where q {\displaystyle q} is the electron charge, r {\displaystyle \mathbf {r} } is the position of the electron relative to the nucleus, r = | r | {\displaystyle r=|\mathbf {r} |} is the magnitude of the relative position, the potential term is due to the Coulomb interaction, wherein ε 0 {\displaystyle \varepsilon _{0}} is the permittivity of free space and μ = m q m p m q + m p {\displaystyle \mu ={\frac {m_{q}m_{p}}{m_{q}+m_{p}}}} is the 2-body reduced mass of the hydrogen nucleus (just a proton) of mass m p {\displaystyle m_{p}} and the electron of mass m q {\displaystyle m_{q}} . The negative sign arises in the potential term since the proton and electron are oppositely charged. The reduced mass in place of the electron mass is used since the electron and proton together orbit each other about a common centre of mass, and constitute a two-body problem to solve. The motion of the electron is of principal interest here, so the equivalent one-body problem is the motion of the electron using the reduced mass. The Schrödinger equation for a hydrogen atom can be solved by separation of variables.[17] In this case, spherical polar coordinates are the most convenient. Thus, ψ (r , θ , φ) = R (r) Y ℓ m (θ , φ) = R (r) Θ (θ) Φ (φ) , {\displaystyle \psi (r,\theta ,\varphi)=R(r)Y_{\ell }^{m}(\theta ,\varphi)=R(r)\Theta (\theta)\Phi (\varphi),} where R are radial functions and Y l m (θ , φ) {\displaystyle Y_{l}^{m}(\theta ,\varphi)} are spherical harmonics of degree ℓ {\displaystyle \ell } and order m {\displaystyle m} . This is the only atom for which the Schrödinger equation has been solved for exactly. Multi-electron atoms require approximate methods. The family of solutions are:[18] ψ n ℓ m (r , θ , φ) = (2 n a 0) 3 ⋅ (n − ℓ − 1) ! 2 n [(n + ℓ) !] e − r / n a 0 (2 r n a 0) ℓ L n − ℓ − 1 2 ℓ + 1 (2 r n a 0) ⋅ Y ℓ m (θ , φ) {\displaystyle \psi _{n\ell m}(r,\theta ,\varphi)={\sqrt {\left({\frac {2}{na_{0}}}\right)^{3}{\frac {(n-\ell -1)!}{2n[(n+\ell)!]}}}}e^{-r/na_{0}}\left({\frac {2r}{na_{0}}}\right)^{\ell }L_{n-\ell -1}^{2\ell +1}\left({\frac {2r}{na_{0}}}\right)\cdot Y_{\ell }^{m}(\theta ,\varphi)} where a 0 = 4 π ε 0 ℏ 2 m q q 2 {\displaystyle a_{0}={\frac {4\pi \varepsilon _{0}\hbar ^{2}}{m_{q}q^{2}}}} is the Bohr radius, L n − ℓ − 1 2 ℓ + 1 (⋯) {\displaystyle L_{n-\ell -1}^{2\ell +1}(\cdots)} are the generalized Laguerre polynomials of degree n − ℓ − 1 {\displaystyle n-\ell -1} , n , ℓ , m {\displaystyle n,\ell ,m} are the principal, azimuthal, and magnetic quantum numbers respectively, which take the values n = 1 , 2 , 3 , ... , {\displaystyle n=1,2,3,\dots ,} ℓ = 0 , 1 , 2 , ... , n − 1 , {\displaystyle \ell =0,1,2,\dots ,n-1,} m = − ℓ , ... , ℓ . {\displaystyle m=-\ell ,\dots ,\ell .} Approximate solutions It is typically not possible to solve the Schrödinger equation exactly for situations of physical interest. Accordingly, approximate solutions are obtained using techniques like variational methods and WKB approximation. It is also common to treat a problem of interest as a small modification to a problem that can be solved exactly, a method known as perturbation theory. Semiclassical limit One simple way to compare classical to quantum mechanics is to consider the time-evolution of the expected position and expected momentum, which can then be compared to the time-evolution of the ordinary position and momentum in classical mechanics.[19]:302 The quantum expectation values satisfy the Ehrenfest theorem. For a one-dimensional quantum particle moving in a potential V {\displaystyle V} , the Ehrenfest theorem says m d d t ⟨ x ⟩ = ⟨ p ⟩ ; d d t ⟨ p ⟩ = − ⟨ V ′ (X) ⟩ . {\displaystyle m{\frac {d}{dt}}\langle x\rangle =\langle p\rangle ;\quad {\frac {d}{dt}}\langle p\rangle =-\left\langle V'(X)\right\rangle .} Although the first of these equations is consistent with the classical behavior, the second is not: If the pair ⟨ (X) , ⟨ P ⟩ ⟩ {\displaystyle (\langle X\rangle ,\langle P\rangle)} were to satisfy Newton's second law, the right-hand side of the second equation would have to be

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