Wave Equation
• Wave-particle duality

• Quantized modes

• Schrödinger equation

• One-dimensional solutions

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• Dirac equation
Wave-particle duality: Matter waves

The major breakthrough occurred in 1923 when a French graduate student, Prince Louis de Broglie, wrote in his thesis the suggestion that, if electromagnetic radiation can have both particle (photon) and wave-like properties, perhaps all forms of matter exhibit this wave-particle duality. That is, he suggested that the wave-particle duality was universal, and therefore matter waves should exist.

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Wave-particle duality: Matter waves

It is convention to express $\nu$, $\lambda$, and $\hbar$ in terms of angular frequency $\omega$:

$$\omega = 2\pi \nu$$

wave number $k$:

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

and $\hbar$; called "h-bar"

$$\hbar = \frac{\hbar}{2\pi}$$

Using these, the de Broglie relations are rewritten as:

\begin{align*}
\mathcal{E} &= \hbar \omega \\
\mathbf{p} &= \hbar \mathbf{k}
\end{align*}

Note that the wavenumber is a vector that points in the direction of the wave as does the momentum. Thus $\mathbf{k}$ has three components, $k_x$, $k_y$, and $k_z$. 
Wave-particle duality: Matter waves

de Broglie noticed a remarkable fact that the Bohr quantization hypothesis was equivalent to requiring standing waves for the electrons orbiting the atom. That is, the Bohr hypothesis:

\[ \mathbf{l} = m \mathbf{v} \times \mathbf{r} = \mathbf{p} \times \mathbf{r} = n \frac{\hbar}{2\pi} = n\hbar \]

where \( n \) is a positive integer. Using the de Broglie relation that \( p = \frac{\hbar}{\lambda} \) for a circular orbit gives:

\[ \frac{\hbar}{\lambda} r = n \frac{\hbar}{2\pi} \]

that is,

\[ n\lambda = 2\pi r \]

As shown in figure 2, this is equivalent to requiring standing waves having an integral number of wavelengths around the circumference of the orbit. Here was a rational and deductive explanation of the Bohr hypothesis. The real test, however, is that if particles have wave-like properties then it should be possible to observe wave-like behavior using a beam of particles analogous to what is observed with light.
Use of complex number representation of wave functions

It is easier to employ the complex form when describing sinusoidal wave motion.

\[ Ae^{i\theta} = A(\cos \theta + i \sin \theta) \]

It is much easier to add or subtract exponents of the exponentials rather than take products of sines and cosines.

The real part of \( Ae^{i\theta} \) projects out \( A\cos \theta \), while the imaginary part projects out the corresponding \( A\sin \theta \) function. The simplest travelling wave in one dimension, \( x \), of the form

\[ \Psi = A\cos(k_x x - \omega t) \]

can be rewritten in the exponential form as:

\[ \Psi = Ae^{i(k_x x - \omega t)} \]
Copenhagen Interpretation

Schrodinger appeared as a saviour to Einstein and Planck because he eliminated the irrational features of the Bohr atom. However, it still left the basic problem of how can particles or light have the contradictory particle and wave-like behavior. The solution to this contradiction was suggested by Max Born, who saw a probabilistic connection between the wave and particle. This idea was promoted strongly by Niels Bohr. The basic idea, which now is generally accepted, is that the intensity of the electron wave, that is the amplitude squared, gives the probability of finding the electron at any point in space or time.
Copenhagen Interpretation

A particle is described by a wavepacket travelling with the velocity of the particle. The probability of finding the particle at any point is proportional to the square of the wavepacket amplitude. Thus if the wavefunction is described by the function $\Psi(xyzt)$, then the Copenhagen Interpretation of wave-particle duality is that the intensity of the wave, $|\Psi(x, y, z, t)|^2$ gives the probability distribution function $P(xyzt)$ of finding the particle at any location, $x, y, z$, at time $t$. That is

$$P(xyzt) = |\Psi(xyzt)|^2$$

Quantum mechanics is probabilistic, that is, it does not determine the exact behavior of the particle, it only tells you the probability of finding the particle with certain conditions. Assuming that the probability of finding the particle somewhere is unity, implies that the integral of the probability over all space is unity.

$$\int_{all\ space} |\Psi|^2 d\tau = 1$$
Expectation values of observables

Wave motion implies that exact specifications for a particle cannot be determined simultaneously, only the probability distribution is measurable. Thus one can only determine expectation values, that is average values, for observables. For example the average value of position $x$ is given by evaluating the probability distribution with $x$. That is, the expectation value of $x$ is:

$$\langle x \rangle = \int x |\Psi(x, t)|^2 \, dx$$

Similarly one can evaluate the expectation value for $x^2$:

$$\langle x^2 \rangle = \int x^2 |\Psi(x, t)|^2 \, dx$$

These can be used to calculate the standard deviation of the spread of the average value $\langle x \rangle$. That is:

$$\sigma(x) = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

Note that $\sigma(x)$ is a non-zero positive number for a non-localized probability distribution. The expectation values of time, linear momentum, angular momentum, energy, or other possible observables can be evaluated if the wavefunction is known, providing a method for relating physical observables in quantum physics.
General uncertainty relation for wave amplitudes and intensities

\[ \sigma_I(t) \cdot \sigma_I(\omega) \geq \frac{1}{2} \]

\[ \sigma_I(x) \cdot \sigma_I(k_x) \geq \frac{1}{2} \]

\[ \sigma_I(y) \cdot \sigma_I(k_y) \geq \frac{1}{2} \]

\[ \sigma_I(z) \cdot \sigma_I(k_z) \geq \frac{1}{2} \]
Heisenberg Uncertainty Principle

The above uncertainty principles apply to all forms of wave motion, be they, sound waves, water waves, electromagnetic waves, or matter waves. In the case of matter waves, the de Broglie relations \( E = \hbar \omega \) and \( \vec{p} = \hbar \vec{k} \) can be inserted into the wave uncertainty principles to give the Heisenberg Uncertainty Principle:

\[
\begin{align*}
\sigma_I(t) \cdot \sigma_I(E) & \geq \frac{\hbar}{2} \\
\sigma_I(x) \cdot \sigma_I(p_x) & \geq \frac{\hbar}{2} \\
\sigma_I(y) \cdot \sigma_I(p_y) & \geq \frac{\hbar}{2} \\
\sigma_I(z) \cdot \sigma_I(p_z) & \geq \frac{\hbar}{2}
\end{align*}
\]

(Heisenberg Uncertainty Principle)
Quantized modes

Confinement of a wave to a restricted range in position leads to:

- **Quantized modes**
- **Minimum zero-point motion**

Consider the one dimensional case. For a localized region of \( x \), discrete values of the corresponding wavenumber \( k_x = \frac{2\pi}{\lambda_x} \) occur. For example, the discrete solutions on a violin string of length \( L \) have possible wavelengths, \( \lambda_n = \frac{2L}{n} \) where \( n \) is a positive integer, \( n \geq 1 \). That is, the wavenumber has quantized solutions \( k_n = \frac{n\pi}{L} \) where \( n \) is the corresponding integer quantum number. That is, solutions are separated by multiples of \( \Delta k_x = \frac{\pi}{L} \). The separation between adjacent quantized solutions goes to zero, that is becomes continuous, when \( L \to \infty \).

If the wave has a fixed velocity \( v \), then since \( \omega = vk \), quantized values of \( k \) correspond to quantized frequencies \( \omega \). For matter waves, quantized values of \( k_x \) implies quantized \( p_x = \hbar k_x \), and consequently quantized values of kinetic energy.
Quantum Number

A one-dimensional wave leads to a single integer quantum number \( n \) characterizing the solutions. A three-dimensional box can have three independent standing waves for each independent degree of freedom, i.e. the \( x \), \( y \), and \( z \) directions. Standing wave systems for each of these three independent spatial degrees of freedom has an associated quantum number characterizing the number of half wavelengths fitting along that dimension. Thus there is one quantum number for every degree of freedom of a quantal system.
Zero-point energy

Confinement of a particle, of mass m, within ±\(\sigma(x)\) of a fixed location implies that there is a corresponding uncertainty in the momentum

\[
\sigma(p) \geq \frac{\hbar}{2\sigma(x)}
\]

Now the variance in p is given by

\[
\sigma(p)^2 = \langle p^2 \rangle - \langle p \rangle^2
\]

Since the fixed location implies that \(\bar{p} = 0\), then

\[
\langle p^2 \rangle = \sigma(p)^2 \geq \left( \frac{\hbar}{2\sigma(x)} \right)^2
\]

Since the kinetic energy is given by:

\[
\text{Kinetic energy} = \frac{p^2}{2m} \geq \frac{\hbar^2}{8m\sigma(x)^2}
\]

(Zero-point energy)
The Schrödinger equation was the first useful quantum wave equation. However, it is *applicable only to non-relativistic cases*. As opposed to classical physics, where the wave equation can be derived from first principles, in quantum physics the wave equation is obtained by a plausibility argument based on classical physics and the de Broglie hypotheses. Inserting the de Broglie relations

\[
\begin{align*}
\mathcal{E} &= \hbar \omega \\
px &= \hbar k_x.
\end{align*}
\]

into the simplest form of a travelling wave in one dimension gives:

\[
\Psi' = Ae^{\frac{i}{\hbar}(pxx-\mathcal{E}t)}
\]
Schrödinger Equation

\[ \Psi' = A e^{\frac{i}{\hbar} (p_xx - \mathcal{E}t)} \]

The relativistic energy \( \mathcal{E} = E + m_0c^2 \) where \( E \) is the kinetic energy. The wave function can be written as

\[ \Psi' = A e^{\frac{i}{\hbar} (p_xx - Et)} e^{-\frac{i}{\hbar} m_0c^2 t} = \Psi e^{-\frac{i}{\hbar} m_0c^2 t} \]

where

\[ \Psi = A e^{\frac{i}{\hbar} (p_xx - Et)} \]

The exponential term \( e^{-\frac{i}{\hbar} m_0c^2 t} \) can be ignored, since it only introduces an unimportant phase factor that has no influence on the probability, that is,

\[ |\Psi'|^2 = |\Psi|^2 \]
Schrödinger Equation

\[ \Psi = A e^{i \frac{p_x x - Et}{\hbar}} \]

Consider the wavefunction \( \Psi(x, t) \) in one dimension. Note that differentials of \( \Psi(x, t) \) are:

\[ \frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} E \Psi \]

That is:

\[ E \Psi = i \hbar \frac{\partial \Psi}{\partial t} \]

Also:

\[ \frac{\partial^2 \Psi}{\partial x^2} = -\frac{p_x^2}{\hbar^2} \Psi \]

That is:

\[ p_x^2 \Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \]
Time-dependent Schrödinger equation

Schrödinger developed a non-relativistic wave equation based on the fact that:

\[ E \Psi = i\hbar \frac{\partial \Psi}{\partial t} \]

\[ p_x^2 \Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2} \]

where \( U \) is the potential energy. Since \( \left( \frac{v}{c} \right)^2 \) is \( 10^{-5} \) for electron orbits in atoms, and \( 10^{-3} \) for protons in the nucleus, the non-relativistic equation is a reasonable approximation for solving many problems in atomic and nuclear physics.

Substituting the above differential expressions for \( E \) and \( p^2 = p_x^2 + p_y^2 + p_z^2 \), gives Schrödinger’s time-dependent equation in three dimensions:

\[ E \Psi = i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + U \Psi \]

(Time dependent Schrödinger equation)
Time-dependent Schrödinger equation

\[ E\Psi = i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + U\Psi \]

(Time dependent Schrodinger equation)

Note that the following facts were used in developing this equation:

- de Broglie-Einstein relations \( \mathcal{E} = \hbar \omega, \quad \vec{p} = \hbar \vec{k} \).
- Non-relativistic relation \( E = \frac{p^2}{2m} + U \)
- Ignored consequences of the phase factor \( e^{-\frac{i}{\hbar} m_0 c^2 t} \)

In general the wavefunction \( \Psi(x, y, z, t) \) is obtained by solving this time-dependent equation for some known potential \( U(x, y, z, t) \).
Time-independent potentials

\[ E\Psi = i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + U\Psi \]

A frequently encountered problem is where the potential is time independent, \( U(x, y, z) \), for which the quantized energy solutions are time independent. For such cases the right-hand side of the time-dependent Schrödinger equation is a function of only the spatial coordinates while the left-hand side is a function only of time. For such a system the two sides are independent and the spatial and time parts of the wavefunction can be separated:

\[ \Psi(x, y, z, t) = \phi(x, y, z)e^{-\frac{i}{\hbar}Et} \]
Time-independent Schrödinger equation

\[ E\Psi = i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + U\Psi \]

\[ \Psi(x, y, z, t) = \phi(x, y, z)e^{-\frac{i}{\hbar}Et} \]

The left-hand side of the equation equals:

\[ i\hbar \frac{\partial \Psi}{\partial t} = i\hbar \phi \frac{\partial e^{-\frac{i}{\hbar}Et}}{\partial t} = E\Psi \]

while the right-hand side gives:

\[ E\phi = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) + U\phi \]

(Time independent Schrodinger equation)

where the time-dependent term of \( \Psi \), that is, \( e^{-\frac{i}{\hbar}Et} \), on both sides cancels. This equation is easier to solve than is Schrödinger’s time-dependent equation.
Schrödinger equation: solution restrictions

\[ E\phi = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} \right) + U\phi \]

**Wavefunction normalization**

The wavefunction must be correctly normalized, that is the probability of finding the particle over all space must be unity, that is:

\[
\int_{\text{all space}} |\phi|^2 \, d\tau = 1 \quad (\text{Wavefunction normalization.})
\]

This fixes the normalization of the wavefunction.

**Continuity**

The wavefunction must be a well-behaved function for which \(\frac{\partial \Psi}{\partial t}, \frac{\partial^2 \phi}{\partial x^2}, \frac{\partial^2 \phi}{\partial y^2},\) and \(\frac{\partial^2 \phi}{\partial z^2}\) all exist. This implies that:

\[\phi, \text{ is continuous} \]

\[\nabla \phi \text{ is continuous}\]

That is, \(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y},\) and \(\frac{\partial \phi}{\partial z}\) all are continuous, if the potential energy function \(U\) is not infinite.
Infinite one-dimensional square well

Consider a mass $m$ contained in a one-dimensional box with $U = 0$ for $0 \leq x \leq L$, and $U = \infty$ outside this region. The time independent Schrödinger equation for $0 \leq x \leq L$ is:

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

since $U = 0$. The wavefunction $\phi$ must be zero outside of the box because then the potential $U = \infty$. Thus $\phi(x)$ must equal zero at the walls of the box, $x = 0$ and $x = L$. Therefore, as for waves on a violin string, the solutions of $\phi = A\sin(kx)$ for $0 \leq x \leq L$ are:

$$\phi_n = A_n \sin(k_n x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

where $n$ is an integer quantum number. The constant $A_n$ has been normalized by requiring $\int_0^L \phi_n^2 \, dx = 1$, while the wavenumber $k_n$ is given by:

$$k_n = \frac{2\pi}{\lambda_n} = n \frac{\pi}{L},$$

that is,

$$\lambda_n = \frac{2L}{n}$$

Substitution of $\phi_n$ into the Schrödinger equation gives corresponding energies:

$$E_n = \frac{\hbar^2}{2m} k_n^2 = n^2 \frac{\hbar^2 \pi^2}{2mL^2}$$
Finite one-dimensional square well

Consider the potential well shown in figure 3, where $U = 0$, for $0 \leq x \leq L$, $U = U_o$ outside of this region of $x$. Thus the Schrödinger equation can be written as:

$$-rac{\hbar^2}{2m} \frac{d^2 \phi}{dx^2} = E \phi \quad (0 \leq x \leq L)$$

$$-rac{\hbar^2}{2m} \frac{d^2 \phi}{dx^2} = (E - U_o) \phi \quad (x \leq 0 \text{ or } x \geq L)$$

Consider possible standing-wave solutions of the form:

$$\phi = Ae^{ikx} + Be^{-ikx}$$

Inserting this into the Schrödinger equation gives inside the potential well, $0 \leq x \leq L$

$$\frac{\hbar^2}{2m} k_1^2 = E$$

and outside the well:

$$\frac{\hbar^2}{2m} k_0^2 = E - U_o$$
Finite square well: Inside well

Thus the solution inside the well is a sinusoidal standing wave with wavenumber:

\[ k_I = \frac{\sqrt{2mE}}{\hbar} \quad \text{(Wavenumber inside well)} \]

That is:

\[ \phi = Ae^{ik_Ix} + Be^{-ik_Ix} = C \sin(k_Ix) \]
Finite square well:

Outside well

The wavenumber outside of the well is given by:

\[ k_0 = \frac{\sqrt{2m(E - U_o)}}{\hbar} \]  (Wavenumber outside well.)

Note that if \( E - U_o \) is positive, that is \( E \) exceeds the depth of the potential, then the solution is sinusoidal with a smaller wavenumber, that is longer wavelength, than inside the potential well. If \( E - U_o \) is negative, that is, \( E < U_o \), then \( \sqrt{2m(E - U_o)} \) is an imaginary number. That is:

\[ k_0 = \frac{i\sqrt{2m(U_o - E)}}{\hbar} = i\beta \]

Thus the solution outside the well now is:

\[ \phi = De^{-\beta x} + Ee^{\beta x} \]

This corresponds to an exponential decay as shown in figure 3.
Finite square well:

The final solutions inside and outside of the well are now obtained using the continuity and normalization requirements, that is:

- Matching the inside and outside values of $\phi$ at the well boundaries $x = 0$ and $x = L$.
- Matching the inside and outside gradients $\frac{d\phi}{dx}$ at the well boundaries $x = 0$ and $x = L$.
- Requiring that $\int_{-\infty}^{\infty} |\phi|^2 \, dx = 1$
Quantum Harmonic Oscillator

\[ U = \frac{1}{2} k x^2 \]

Energy

- \( n = 0 \) with \( E = \frac{1}{2} \hbar \omega_0 \)
- \( n = 1 \) with \( E = \frac{3}{2} \hbar \omega_0 \)
- \( n = 2 \) with \( E = \frac{5}{2} \hbar \omega_0 \)
- \( n = 3 \) with \( E = \frac{7}{2} \hbar \omega_0 \)
Solution of the time-independent Schrödinger equation in three dimensions leads to solutions in three independent directions, each of which has its own quantum number. It is useful to first consider the three-dimensional infinite square well potential since it illustrates important characteristics of solutions of the Schrödinger equation.
Consider the three-dimensional infinite square well potential where \( U(xyz) = 0 \) for \( 0 < x < L, 0 < y < L, 0 < z < L \). Outside this cubical square well \( U(xyz) = \infty \). The wave function solutions to this potential must be zero at the infinite boundaries. Thus the solutions

\[
\Psi(xyz) = A \sin k_1 x \sin k_2 y \sin k_3 z
\]

where the constant \( A \) is given by normalization of the wavefunction. Inserting this solution into Schrödinger’s equation gives energies inside the box of

\[
E = \frac{\hbar^2}{2m} \left( k_1^2 + k_2^2 + k_3^2 \right)
\]

As for the infinite one-dimensional square well, the potential must be zero at the walls, therefore the only possible solutions are quantized with

\[
k_1 = n_1 \frac{\pi}{L} \\
k_2 = n_2 \frac{\pi}{L} \\
k_3 = n_3 \frac{\pi}{L}
\]

where \( n_I \geq 1 \) and integer. Therefore

\[
E = \frac{\hbar^2 \pi^2}{2mL^2} \left( n_1^2 + n_2^2 + n_3^2 \right)
\]
Three-dimensional infinite square well

\[ E = \frac{\hbar^2 \pi^2}{2mL^2} \left( n_1^2 + n_2^2 + n_3^2 \right) \]

The lowest energy, that is, ground state, for this cubical infinite square well is

\[ E_{1,1,1} = \frac{3\hbar^2 \pi^2}{2mL^2} \]

The first excited state can be made three different ways, each having the same energy. That is

\[ E_{2,1,1} = E_{1,2,1} = E_{1,1,2} = \frac{6\hbar^2 \pi^2}{2mL^2} \]

where, for example, the 2,1,1 wavefunction is

\[ \Psi_{2,1,1} = A \sin \frac{2\pi x}{L} \sin \frac{\pi y}{L} \sin \frac{\pi z}{L} \]

Note that these three solutions are degenerate, that is, they have the same excitation energy, if the box is the same size in the three directions. This often happens in quantum physics. This degeneracy is removed if the box has different sizes in the three directions as shown in figure 5. This happens in deformed nuclei that are football shaped, that is, where one axis may be significantly longer than the other two axes.
Several forces in physics are spherically symmetric, that is the force depends only on the radial distance, not angle. This is true of the gravitational force, Coulomb force and nuclear force. For such forces it is better to use the orthogonal spherical coordinates, \(r, \theta,\) and \(\varphi\) rather than \(x, y, z\), since then the spherically-symmetric potential energy \(U\) is only a function of the one variable \(r\). The angles \(\theta\) and \(\varphi\) are the latitude and longitude on the surface of a sphere at a given radius. Instead of associating quantum numbers describing the \(x, y,\) and \(z\) directions, one uses quantum numbers characterizing waves that are solutions in the \(r, \theta\) and \(\varphi\) directions.

The Schrödinger equation in spherical coordinates is:

\[
-\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \phi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \phi}{\partial \varphi^2} \right] + U \phi = E \phi
\]

For a spherically-symmetric potential, the solution separates into the form:

\[
\phi(r\theta\varphi)_{nlm} = R_{nl}(r) \Theta_l(\theta) \Phi_m(\varphi)
\]
Spherically-symmetric potentials

\[ \phi(r \theta \varphi)_{nlm} = R_{nl}(r) \Theta_l(\theta) \Phi_m(\varphi) \]

The corresponding quantum numbers are called; \( n \) for \( r \), \( l \) for \( \theta \), and \( m \) for \( \varphi \). Standing waves in \( \theta \) and \( \varphi \) requires that the pattern repeat after one complete revolution around the surface of the sphere. Note that if \( U \) is spherically symmetric, then the angular part of Schrödinger’s equation, is contained completely within the curly brackets, and the solutions are independent of the radial form of the potential well.

Schrödinger showed that the orbital angular momentum \( \mathbf{L} = \mathbf{r} \times \mathbf{p} \) of a particle described by the angular wavefunction \( \Theta_l(\theta) \Phi_m(\varphi) \) has an angular momentum \( L \) of:

\[ L = \hbar \sqrt{l(l + 1)} \]

where \( l \) is called the orbital angular momentum quantum number.

Also Schrödinger showed that the projection of this orbital angular momentum on the \( z \) axis \( L_z \) for \( \Theta_l(\theta) \Phi_m(\varphi) \) equals:

\[ L_z = m \hbar \]

where \( m \) is called the magnetic quantum number. Note that the magnetic quantum number can take values between \( \pm l \). That is;

\[-l \leq m \leq +l\]
Next lecture will use Schrödinger’s equation in this form to solve the hydrogen atom. Schrödinger derived Bohr’s quantization of the orbital angular momentum from his wave equation without resorting to ad hoc assumptions. For such spherically-symmetric potentials the binding energies are independent of $\theta$ and $\varphi$, the energy depends only on the radial quantum number $n$, and $l$ due to centripetal effects. In general the solution of the radial part of the Schödinger equation can be difficult and usually requires use of a computer.
Erwin Schrödinger

The first of Schrödinger’s six great papers establishing the theory once known as wave mechanics was written during a two-week vacation at Christmas, 1925. According to a recent biography,*

Erwin wrote to “an old girl friend in Vienna” to join him in Arosa, while Anny [his wife] remained in Zürich. Efforts to establish the identity of this woman have so far been unsuccessful. Like the dark lady who inspired Shakespeare’s sonnets, the lady of Arosa may remain forever mysterious. We know that she was not Lotte or Irene [or] Felicie. Whoever may have been his inspiration, the increase in Erwin’s powers was dramatic, and he began a twelve-month period of sustained creative activity that is without parallel in the history of physics.

Schrödinger’s first paper on wave mechanics, written from his love nest in the Swiss Alps, begins with a bang:

In this communication, I wish first to show in the simplest case of the hydrogen atom that [Bohr’s] rules for quantization can be replaced by another requirement, in which mention of “whole numbers” no longer occurs. Instead the integers occur in the same natural way as the integers specifying the number of nodes in a vibrating string. The new conception can be generalized, and I believe it touches the deepest meaning of the quantum rules.

*Walter Moore, Schrödinger, Life and Thought (Cambridge Univ. Press, 1989)
Schrödinger tried unsuccessfully to develop a relativistic wave equation but failed. It was Dirac, in 1928, who finally derived the ultimate relativistic wave equation. It is complicated to use and physicists only use it when the non-relativistic approach is inapplicable. What is remarkable about the Dirac equation is that it predicts:

- electron spin,
- negative-energy states

Dirac had to conclude that the negative energy states, illustrated in the figure, were in fact completely filled with electrons. A hole in this negative sea of electrons will behave like a positive electron. Raising an electron from this negative sea produces a free electron plus a positive hole, which we call a positron. Dirac realized immediately that the positive hole has to have the mass of the electron, that is, it is not a proton. Oppenheimer, who later led the US nuclear bomb project, showed that the negative-energy solutions actually correspond to positive-energy states of positive particles. Dirac’s concept of a sea of electrons filling all of the negative states was an unnecessary edifice, one really just has positive and negative electrons. Thus the Dirac equation predicts four states of the electron: spin up and spin down for both positive and negative electrons. This seemingly wild idea of positive electrons was confirmed in 1932 when Anderson discovered the positron. He observed electrons deflected in both directions in a cloud chamber that was between the poles of a large magnet.
Particles and anti-particles

The positron is called the antiparticle of the electron. Soon after Anderson’s discovery, Dirac realized that there should also be an antiparticle to the proton. In fact, an antiparticle exists for every type of particle. The masses of particles, and their corresponding antiparticle, have been measured to be identical to a few parts per billion, while the charge and magnetic properties are identical in value but opposite in sign. A particle and its antiparticle can annihilate each other and the energy is released as electromagnetic energy or some other particle-antiparticle pair as long as energy conservation is satisfied. Using Einstein’s equation \( E = mc^2 \) to compute that the rest mass of an electron corresponds to 0.511 MeV of energy. To create an electron-positron pair requires at least twice 0.511 MeV, that is greater than 1.022 MeV of energy.

Antiprotons were not observed until the Bevatron accelerator was built at Berkeley in the 1950’s. If a proton annihilates an antiproton, they release an energy of 1.876.5 GeV plus the kinetic energy. Some people surmise that maybe antigalaxies exist. Think what would happen to our galaxy if it collided with another galaxy made of antimatter, the energy released would be truly astronomical. If an antiworld piece of matter the size of the earth hit the earth the annihilation energy would be \( 10^{42} \) J, that is the energy radiated by the sun during the past 30 million years.
Dirac theory

The Dirac theory was expanded in the 1940’s to include electromagnetism, this extension of quantum theory is called quantum electrodynamics, QED. It is a remarkably successful theory. For example, the magnetic moment of the proton is predicted to 10 decimal places and has been measured to be this value with a similar precision. The Dirac equation is more difficult to solve than the non-relativistic Schrodinger equation. Fortunately, relativistic effects are generally negligible for atomic and molecular systems and thus the Schrödinger equation is an adequate approximation for most applications of wave mechanics.
The Schrödinger equation led to an amazing advance in our knowledge of quantum mechanics and the hydrogen atom. The next advances needed are the introduction of spin and the Pauli Exclusion Principle. These allow an explanation of both single and multi-electron atoms, molecular systems and nuclei.