Schrodinger's Wave Simulation(Using Python)

A Project Report

Submitted By

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Project Abstract

Project Idea: Schrödinger introduced a mathematical function ψ which is the variable quantity associated with the moving particle and is a complex function of the space coordinates of the particle and the time. Ψ is called the 'wave function' as it characterizes the de Broglie waves associated with the particle. It is postulated that ψ has the form of the solution of the classical wave equation.
Using the wave function he derived the equation which is given as

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

Coding Using Python: Python is currently the best data visualization language available to us. Plotting a probability distribution curve will be much easier using Python. Also, apart from effortless syntax Python offers a variety of tools that help us to visualize data precisely.

My Take On The Project:
Quantum Mechanics is the approaching future of Physics, which may revolutionize Science and Technology. Schrödinger's Wave Equation is the foremost Quantum theory put forth by Schrödinger, and simulating it will be my way of visualizing the wave equation.

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Introduction To Quantum Mechanics

Introduction:

Quantum Mechanics is a science dealing with the behaviour of matter and light on the atomic and subatomic scale. It attempts to describe and account for the properties of molecules and atoms and their constituents—electrons, protons, neutrons, and other more esoteric particles such as quarks and gluons. These properties include the interactions of the particles with one another and with electromagnetic radiation (i.e., light, X-rays, and gamma rays). The behaviour of matter and radiation on the atomic scale often seems peculiar, and the consequences of quantum theory are accordingly difficult to understand and believe. Its concepts frequently conflict with common-sense notions derived from observations of the everyday world. There is no reason, however, why the behaviour of the atomic world should conform to that of the familiar, large-scale world. It is important to realize that quantum mechanics is a branch of physics and that the business of physics is to describe and account for the way the world—on both the large and the small scale—actually is and not how one imagines it or would like it to be. The study of quantum mechanics is rewarding for several reasons. First, it illustrates the essential methodology of physics. Second, it has been enormously successful in giving correct results in practically every situation to which it has been applied. There is, however, an intriguing paradox. In spite

of the overwhelming practical success of quantum mechanics, the foundations of the subject contain unresolved problems—in particular, problems concerning the nature of measurement. An essential feature of quantum mechanics is that it is generally impossible, even in principle, to measure a system without disturbing it; the precise nature of this disturbance and the exact point at which it occurs are obscure and controversial.

Thus, quantum mechanics attracted some of the ablest scientists of the 20th century, and they erected what is perhaps the finest intellectual edifice of the period.

Early developments

Planck's radiation law:

In 1900 the German theoretical physicist Max Planck made a bold suggestion. He assumed that the radiation energy is emitted, not continuously, but rather in discrete packets called quanta. The energy E of the quantum is related to the frequency ν by $E = h\nu$. The quantity h, now known as Planck's constant, is a universal constant with the approximate value of 6.62607×10^{-34} joule·second. Planck showed that the calculated energy spectrum then agreed with observation over the entire wavelength range.

Einstein and the photoelectric effect:

In 1905 Einstein extended Planck's hypothesis to explain the photoelectric effect, which is the emission of electrons by a metal surface when it is irradiated by light or more energetic photons. The kinetic energy of the emitted electrons depends on the frequency ν of the radiation, not on its intensity; for a given metal, there is a threshold frequency ν_o below which no electrons are emitted.

Emission takes place as soon as the light shines on the surface; there is no detectable delay. Einstein showed that these results can be explained by two assumptions: that light is composed of corpuscles or photons, the energy of which is given by Planck's relationship, and that an atom in the metal can absorb either a whole photon or nothing. Part of the energy of the absorbed photon frees an electron, which requires a fixed energy W, known as the work function of the metal; the rest is converted into the kinetic energy $m_e u^2/2$ of the emitted electron (m_e is the mass of the electron and u is its velocity). Thus, the energy relation is

$$h\nu = W + \frac{m_e u^2}{2}.$$

If ν is less than ν_o, where $h\nu_o = W$, no electrons are emitted. Not all of the experimental results mentioned above were known in 1905, but all of Einstein's predictions have been verified since.

Bohr's theory of the atom:

A major contribution to the subject was made by Niels Bohr of Denmark, who applied the quantum hypothesis to atomic spectra in 1913. The spectra of light emitted by gaseous atoms had been studied extensively since the mid-19th century. It was found that radiation from gaseous atoms at low pressure consists of a set of discrete wavelengths. This is quite unlike the radiation from a solid, which is distributed over a continuous range of wavelengths. The set of discrete wavelengths from gaseous atoms is known as a line spectrum, because the radiation (light) emitted consists of a series of sharp lines. The wavelengths of the lines are characteristic of the element and may form extremely complex patterns. The simplest spectra are those of atomic hydrogen and the alkali atoms (e.g., lithium, sodium, and potassium). For hydrogen, the wavelengths λ are given by the empirical formula

$$\frac{1}{\lambda} = R_\infty \left(\frac{1}{m^2} - \frac{1}{n^2} \right),$$

The Uncertainity Principle

Uncertainty principle, also called Heisenberg uncertainty principle or indeterminacy principle, statement, articulated (1927) by the German physicist Werner Heisenberg, that the position and the velocity of an object cannot both be measured exactly, at the same time, even in theory. The very concepts of exact position and exact velocity together, in fact, have no meaning in nature.

Ordinary experience provides no clue of this principle. It is easy to measure both the position and the velocity of, say, an automobile, because the uncertainties implied by this principle for ordinary objects are too small to be observed. The complete rule stipulates that the product of the uncertainties in position and velocity is equal to or greater than a tiny physical quantity, or constant ($h/(4\pi)$, where h is Planck's constant, or about 6.6×10^{-34} joule-second). Only for the exceedingly small masses of atoms and subatomic particles does the product of the uncertainties become significant.

Any attempt to measure precisely the velocity of a subatomic particle, such as an electron, will knock it about in an unpredictable way, so that a simultaneous measurement of its position has no validity. This result has nothing to do with inadequacies in the measuring instruments, the technique, or the observer; it arises out of the intimate connection in nature between particles and waves in the realm of subatomic dimensions.

All these events lead up to apprehending the Schrodinger's Equation.

The Schrodinger's Wave Equation

The Schrödinger equation is a linear partial differential equation that governs the wave function of a quantum-mechanical system.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

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".

At the same time that Schrödinger proposed his time-independent equation to describe the stationary states, he also proposed a time-dependent equation to describe how a system changes from one state to another. By replacing the energy E in Schrödinger's equation with a time-derivative operator, he generalized his wave equation to determine the time variation of the wave function as well as its spatial variation. The time-dependent Schrödinger equation reads

$$-\frac{\hbar^2}{2m_e}\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+V(x,\,y,\,z)\Psi=i\hbar\frac{\partial\Psi}{\partial t}.$$

The quantity i is the square root of -1. The function Ψ varies with time t as well as with position x, y, z. For a system with constant energy, E, Ψ has the form

$$\Psi(x,\,y,\,z,\,t)=\Psi(x,\,y,\,z)\exp\left(-\frac{iEt}{\hbar}\right),$$

where exp stands for the exponential function, and the time-dependent Schrödinger equation reduces to the time-independent form.

The probability of a transition between one atomic stationary state and some other state can be calculated with the aid of the time-dependent Schrödinger equation. For example, an atom may change spontaneously from one state to another state with less energy, emitting the difference in energy as a photon with a frequency given by the Bohr relation. If electromagnetic radiation is applied to a set of atoms and if the frequency of the radiation matches the energy difference between two stationary states, transitions can be stimulated. In a stimulated transition, the energy of the atom may increase—i.e., the atom may absorb a photon from the radiation—or the energy of the atom may decrease, with the emission of a photon, which adds to the energy of the radiation. Such stimulated emission processes form the basic mechanism for the operation of lasers. The probability of a transition from one state to another depends on the values of the l, m, m_s quantum numbers of the initial and final states. For most values, the transition probability is effectively zero. However, for certain changes in the quantum numbers, summarized as selection rules, there is a finite probability. For example, according to one important selection rule, the l value changes by unity because photons have a spin of 1. The selection rules for radiation relate to the angular momentum properties of the stationary states. The absorbed or emitted photon has its own angular momentum, and the selection rules reflect the conservation of angular momentum between the atoms and the radiation.

Harmonic Oscillator:

The quantum harmonic oscillator is the quantum-mechanical analog of the classical harmonic oscillator. Because an arbitrary smooth potential can usually be approximated as a harmonic potential at the vicinity of a stable equilibrium point, it is one of the most important model systems in quantum mechanics. Furthermore, it is one of the few quantum-mechanical systems for which an exact, analytical solution is known.

Applications Of Quantum Mechanics

As has been noted, quantum mechanics has been enormously successful in explaining microscopic phenomena in all branches of physics. The two phenomena described in this section are examples that demonstrate the quintessence of the theory.

1. The kaon (also called the K^o meson), discovered in 1947, is produced in high-energy collisions between nuclei and other particles. It has zero electric charge, and its mass is about one-half the mass of the proton. It is unstable and, once formed, rapidly decays into either 2 or 3 pi-mesons. The average lifetime of the kaon is about 10^{-10} seconds.
In spite of the fact that the kaon is uncharged, quantum theory predicts the existence of an antiparticle with the same mass, decay products, and average lifetime; the antiparticle is denoted by K^o. During the early 1950s, several physicists questioned the justification for postulating the existence of two particles with such similar properties. In 1955, however, Murray Gell-Mann and Abraham Pais made an interesting prediction about the decay of the kaon. Their reasoning provides an excellent illustration of the quantum mechanical axiom that the wave function Ψ can be a superposition of states; in this case, there are two states, the K^o and K^o mesons themselves.

2. Quantum theory has been used to establish a voltage standard, and this standard has proven to be extraordinarily accurate and consistent from laboratory to laboratory.

If two layers of superconducting material are separated by a thin insulating barrier, a supercurrent (i.e., a current of paired electrons) can pass from one superconductor to the other. This is another example of the tunneling process described earlier. Several effects based on this phenomenon were predicted in 1962 by the British physicist Brian D. Josephson. Demonstrated experimentally soon afterward, they are now referred to as the Josephson effects.

Data Visualization and Python

Data visualization is the process of representing data and information in a visual format such as charts, graphs, and maps to help people better understand and interpret the data. Python is a popular programming language for data visualization due to its flexibility, ease of use, and the availability of many powerful libraries such as Matplotlib, Seaborn, Plotly, and Bokeh.

Matplotlib is a widely used data visualization library in Python that provides a variety of plot types such as line, bar, scatter, and histogram. It is highly customizable and can be used to create publication-quality graphics. Seaborn is another popular library that provides more advanced statistical visualizations such as heat maps, violin plots, and cluster maps. It is built on top of Matplotlib and provides a higher-level interface for creating complex visualizations.

Plotly is a web-based data visualization library that provides interactive plots and dashboards. It can be used to create highly interactive and customizable plots that can be embedded in web applications. Bokeh is another interactive data visualization library that provides a variety of plot types and tools for exploring and analyzing data. It is designed to work with large datasets and

provides a high-performance rendering engine for creating complex visualizations.

In summary, Python provides a wide range of tools and libraries for data visualization that can help users to analyze and interpret their data in a more effective and efficient way. Whether it's creating static charts and graphs or building interactive dashboards and web applications, Python has become an essential tool for data scientists and analysts working in various domains.

Result And Conclusions

The final code performs a simulation of a one-dimensional quantum mechanical system using the time-dependent Schrödinger equation. The simulation is performed in the position basis, where the wavefunction is represented as a complex-valued function of position, psi(x,t).

The plot shows the time evolution of the probability density |psi(x,t)|^2, which represents the probability of finding the particle at position x at time t. The initial Gaussian wavefunction spreads out over time due to the uncertainty principle and eventually settles into a steady state oscillation within the parabolic well potential. In summary, this code provides a simple but useful demonstration of the time evolution of a quantum mechanical system and illustrates some important concepts such as the uncertainty principle and periodic boundary conditions.

Bibliography

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Appendix :

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.animation as animation

# Define spatial grid
x_min = -50
x_max = 50
N = 2000
dx = (x_max - x_min) / (N - 1)
x = np.linspace(x_min, x_max, N)

# Define time grid
T = 10
dt = 0.01
n_steps = int(T / dt)
t = np.linspace(0, T, n_steps) #array of the time steps

# Define potential function
def V(x):
    return 0.5 * x**2


# Define initial wavefunction
def psi_init(x):
    return np.exp(-0.5 * (x)**2)

psi = psi_init(x).astype(complex)

# Define Hamiltonian operator with periodic boundary conditions
def H(psi, x, V, dx):
    psi_fft = np.fft.fft(psi)
    k = np.fft.fftfreq(len(x), dx / (2 * np.pi))
    psi_fft *= np.exp(-1j * 0.5 * k**2 * dt)
    psi_fft *= np.exp(-1j * V(x) * dt)
    psi_new = np.fft.ifft(psi_fft)
```

```
    return psi_new



# Define animation function with periodic boundary conditions
def animate(i):
    psi_new = H(psi, x, V, dx)
    psi_new /= np.sqrt(np.sum(np.abs(psi_new)**2) * dx)
    psi_new[0] = psi_new[-2] # Set periodic boundary condition at
x_min
    psi_new[-1] = psi_new[1] # Set periodic boundary condition at
x_max
    line.set_ydata(np.abs(psi_new)**2)
    psi[:] = psi_new
    return line,


# Set up plot
fig, ax = plt.subplots()
ax.set_xlim(x_min, x_max)
ax.set_ylim(0, 0.5)
ax.set_xlabel('x')
ax.set_ylabel('|psi(x,t)|^2')
ax.set_facecolor('black')
line, = ax.plot(x, np.abs(psi)**2, c='red')

# Create animation
ani = animation.FuncAnimation(fig, animate, frames=n_steps,
interval=30, blit=True)

# Show animation
plt.show()
```