Schrödinger's Equation

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Contents

1 The Schrödinger Equation

- Schrödinger's Equation:
  - The behavior of the wave function is controlled by a differential eqution called "Schrödinger's equation"
  - The role is similar to Newton's 2nd law
  - It is a second order differential equation
  - Using a free particle, with A as the amplitude, to derive the equation (at a given time $t = t_o$), $\psi(x)$ is:

$$\boxed{\psi(x) = A\sin(kx), \qquad k = \frac{2\pi}{\lambda}}$$

$$\boxed{\frac{d\psi(x)}{dx} = Ak\cos(kx)}$$

$$\boxed{\frac{d^2\psi(x)}{dx} = -Ak^2\sin(kx) = -k^2\psi(x)}$$

  - Using the kinetic energy, $K = \dfrac{p^2}{2m} = \left(\dfrac{\hbar}{\lambda}\right)^2 \dfrac{1}{2m}$

$$K = \frac{\hbar^2 k^2}{2m}$$

  - Thus, we obtain:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = K\psi(x)}$$

  - Using total energy:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)}$$

  - This is the unidimensional, static[1] Schrödinger equation

- Probability density and normalization
  - We defined $P(x)\,dx = |\psi(x)|^2\,dx$
  - $P(x)\,dx$ represents the probability density

$$\int_{x_1}^{x_2} P(x)\,dx \Rightarrow P(x_1 : x_2)$$

[1] time independent

- Is the probability of finding the particle in range x_1 to x_2

$$\int_{-\infty}^{\infty} P(x)\,dx = 1 \;\forall \text{ particles}$$

- This means:

$$\boxed{\int_{-\infty}^{\infty} |\psi(x)|^2\,dx = 1}$$

- The average location of the particle is given by:

$$\boxed{\frac{\sum n_1 x_1 + n_2 x_2 + \cdots + n_i x_i}{\sum n_1 + n_2 + \cdots + n_i}}$$

- On a much smaller interval, we can use:

$$x_{avg} = \frac{\displaystyle\int_{-\infty}^{\infty} xP(x)\,dx}{\displaystyle\int_{-\infty}^{\infty} P(x)\,dx} = \int_{-\infty}^{\infty} x|\psi(x)|^2\,dx$$

- For any function of x, the average is:

$$[f(x)]_{avg} = \int_{-\infty}^{\infty} f(x)|\psi(x)|^2\,dx$$

- Given a case of constant potential energy:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

- Given a case where $E < U_o$ [2]

$$\psi(x) = Ae^{-kx}$$

- Light emission or absorption with quantum wave systems
  - By emitting energy in photons, the particle can move from a higher state to a lower state
  - By absorbing energy from photons, the particle can move from a lower to a higher state
- Infinite vs. Finite Wells
  - Unlike the infinite well, the particle can penetrate the forbidden region

[2] e^{kx} has to be removed because it diverges

- Excited states are more likely to penetrate deeper into the forbidden region

- Two-Dimensional Quantum Wells
  - The potential energy in an infinite potential energy well:

$$U(x,y) = \begin{cases} 0, & 0 \le (x,y) \le L \\ \infty, & \text{otherwise} \end{cases}$$

  - Inside the quantum well:

$$\psi(x,y) = f(x)g(y)$$

  - The boundary conditions are:

$$\begin{array}{ll} \psi(0,y) = 0 & \psi(L,y) = 0 \\ \psi(x,0) = 0 & \psi(x,L) = 0 \end{array}$$

  - This results in the function:

$$\psi(x,y) = A \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi y}{L}\right)$$

  - Using the property of the wave function, we obtain:

$$\int_0^L \int_0^L |\psi(x)|^2 \, dx \, dy = 1$$

$$A = \frac{2}{L}$$

  - This results in:

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^2 + n_y^2)$$

- Degeneracy of Quantum States
  - It happens that two different states give exactly the same energy
  - The two levels (1,2) and (2,1) are degenerate
  - Degeneracy happens when the # of quantum numbers > 1
  - In quantum wells, the # of quantum numbers = # of dimensions

- The Simple Harmonic Oscillator
  - The potential energy is $U(x) = \frac{1}{2}kx^2$
  - Using Newton's law, the frequency is: $\omega_o = \sqrt{\dfrac{k}{m}}$

- The ground state for any particle is $E = \frac{1}{2}\hbar\omega_o$
- The coefficient A can be obtained by normalization:

$$A = \left(\frac{m\omega_o}{\hbar\pi}\right)^{\frac{1}{4}}$$

- Thus, the ground state wave function becomes:

$$\boxed{\psi(x) = \left(\frac{m\omega_o}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{x^2\sqrt{km}}{2\hbar}}}$$