Erwin Schrödinger (1926, Nobel prize 1933)
also spelled Schroedinger
but ~~not~~ Schrodinger

Chapter 40 —

Quantum mechanics (QM) —

Remember: we're working with a quantum particle, with mass m and wavelength λ, and wave number $k = 2\pi/\lambda$.

The Schrödinger equation is the equation of motion for matter waves: it tells where the matter waves are ("wave mechanics"). It therefore defines QM, much as how $F=ma$ defines classical (Newtonian) mechanics.

For any wave, recall (from Chapter 33) that: $\boxed{\dfrac{\partial^2 y}{\partial x^2} = \left(\dfrac{1}{v^2}\right)\dfrac{\partial^2 y}{\partial t^2}}$, where v = wave speed and y = amplitude.

Consider a stationary wave, such as a standing wave:

$y(x) \equiv \Psi(x) = A \sin kx$

Ψ (used for historical reasons) $\equiv$ the wave function = the amplitude of a matter wave.

Then: $d\Psi(x)/dx = kA\cos kx$

And: $d^2\Psi(x)/dx^2 = -k^2 A \sin kx = -k^2\Psi = \dfrac{-2m}{\hbar^2} K \Psi$, where m = mass of the particle.

Here, K = kinetic energy for $v \ll c$, (since by luck electrons in atoms are non-relativistic) $= \frac{1}{2}mv^2 = \dfrac{p^2}{2m} = \dfrac{(\hbar k)^2}{2m}$.

Also: wave number $k = \dfrac{2\pi}{\lambda} = \dfrac{2\pi p}{h} = \dfrac{p}{\hbar}$, since $\lambda = h/p$ for matter waves, and $\hbar \equiv h/(2\pi)$.

$\Rightarrow \dfrac{d^2\Psi}{dx^2} = \dfrac{-2m}{\hbar^2} K\Psi = \dfrac{-2m}{\hbar^2}(E-U)\Psi$, since $\underset{\text{total energy}}{E} = \underset{\text{kinetic energy}}{K} + \underset{\text{potential energy}}{U}$.

$$\therefore \boxed{-\left(\frac{\hbar^2}{2m}\right)\frac{d^2\Psi}{dx^2} + U\Psi = E\Psi}$$

This is the one-dimensional, time-independent, non-relativistic Schrödinger equation: it gives Ψ as a function of x, U, and E, for a particle of mass m.

Max Born (1928, Nobel prize 1954) realized the physical significance of Ψ: $|\Psi(x)|^2$ gives the probability that the particle is at a given location, so: $|\Psi(x)|^2\,dx = p(x)\,dx$.

$\Rightarrow$ The probability of finding the particle (of mass m) between $x=a$ and $x=b$ is: $\boxed{P_{ab} = \displaystyle\int_{x=a}^{b} p(x)\,dx = \int_a^b |\Psi(x)|^2\,dx}$.

Normalization is a calculation aid for integrals like this: the particle must be somewhere between $-\infty < x < +\infty$, so:

$$\int_{-\infty}^{+\infty} p(x)\,dx = \int_{-\infty}^{+\infty} |\Psi(x)|^2\,dx = \underline{1}.$$

The expectation value is the average, or expected, position of the particle:

(The average of x) $\langle x\rangle = \dfrac{\sum_{i=1}^{N} x_i}{N} = \displaystyle\int_{-\infty}^{+\infty} x\,p(x)\,dx \Big/ \underbrace{\int_{-\infty}^{+\infty} p(x)\,dx}_{=1 \text{ by normalization}} = \int_{x=-\infty}^{\infty} x\,|\Psi(x)|^2\,dx$ (Don't forget)

Example — how to use Schrödinger's equation to calculate the wave function (where the matter waves are), given a potential $U(x)$ —

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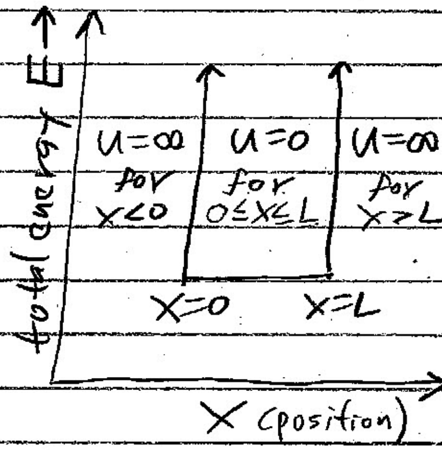
Recall that: $\frac{d^2\psi}{dx^2} = \frac{-2m}{\hbar^2}(E-U)\psi$

$P_{ab} = \int_a^b |\psi(x)|^2 dx$

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

Chapter 40-2 – A particle in a box (one-dimensional case: x only), also called the infinite square well.



This has many uses:
- a 0 or 1 in a computer memory (a qubit),
- a quantum dot in a solar panel,
- an electron in a silicon crystal or metal,
- an electron in an atom (approximately).

The idea is: A quantum particle (e.g. an electron), with mass m and with matter waves, can move freely ($U=0$) inside a box ($0 \le x \le L$), but can't be outside the box, so:

$$U(x) = \begin{cases} 0, & \text{for } 0 \le x \le L \text{ (inside the box)} \\ \infty, & \text{for } x<0 \text{ and } x>L \text{ (outside)} \end{cases}$$

For $0 \le x \le L$ (inside the box), $U=0$, so:

$$\frac{d^2\psi}{dx^2} = \frac{-2m}{\hbar^2}(E-\overset{U=0}{\cancel{0}})\psi = \frac{-2m}{\hbar^2}E\psi = -k^2\psi \text{ (from last class).}$$

Notice that:

$\psi(x) = A \sin kx$ is a solution to $d^2\psi/dx^2 = -k^2\psi$ (from last class),

so: $\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$, since $k = \frac{2\pi}{\lambda} = \frac{2\pi}{2L/n} = \frac{n\pi}{L}$. ✓

Also, since $k^2 = 2mE/\hbar^2$, $E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2 n^2}{2mL^2}$

So: $\boxed{E = \left(\frac{h^2}{8mL^2}\right) n^2, \text{ where } n = 1,2,3\ldots}$

This means that the total energy E of a quantum particle of mass m that is confined in a box (between $0 \le x \le L$) must be quantized: it is not continuous, but can only have specific, discrete values. Electrons in atoms and crystals also can only have discrete amounts of energy, because of their wave properties (and $\psi = 0$ at $x=0$ and $x=L$).

Recall that: $\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}(E-U)\psi$

$P_{ab} = \int_a^b |\psi(x)|^2 dx$

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

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QM particle in a box (1-D case), continued —

From above: $\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$

Normalize, to find A —

$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$, so $\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$,

since $\psi = 0$ outside the box (for $x<0$ and $x>L$)

Solve this integral $\Rightarrow A = \sqrt{2/L}$,

so the wave function is: $\boxed{\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right),\ n = 1, 2, 3 \ldots}$

Draw the wave function ψ and the probability density $|\psi|^2$, noting how $\psi = 0$ at $x=0$ and $x=L$ (at the edges of the box), and for $x<0$ and $x>L$ (outside the box):