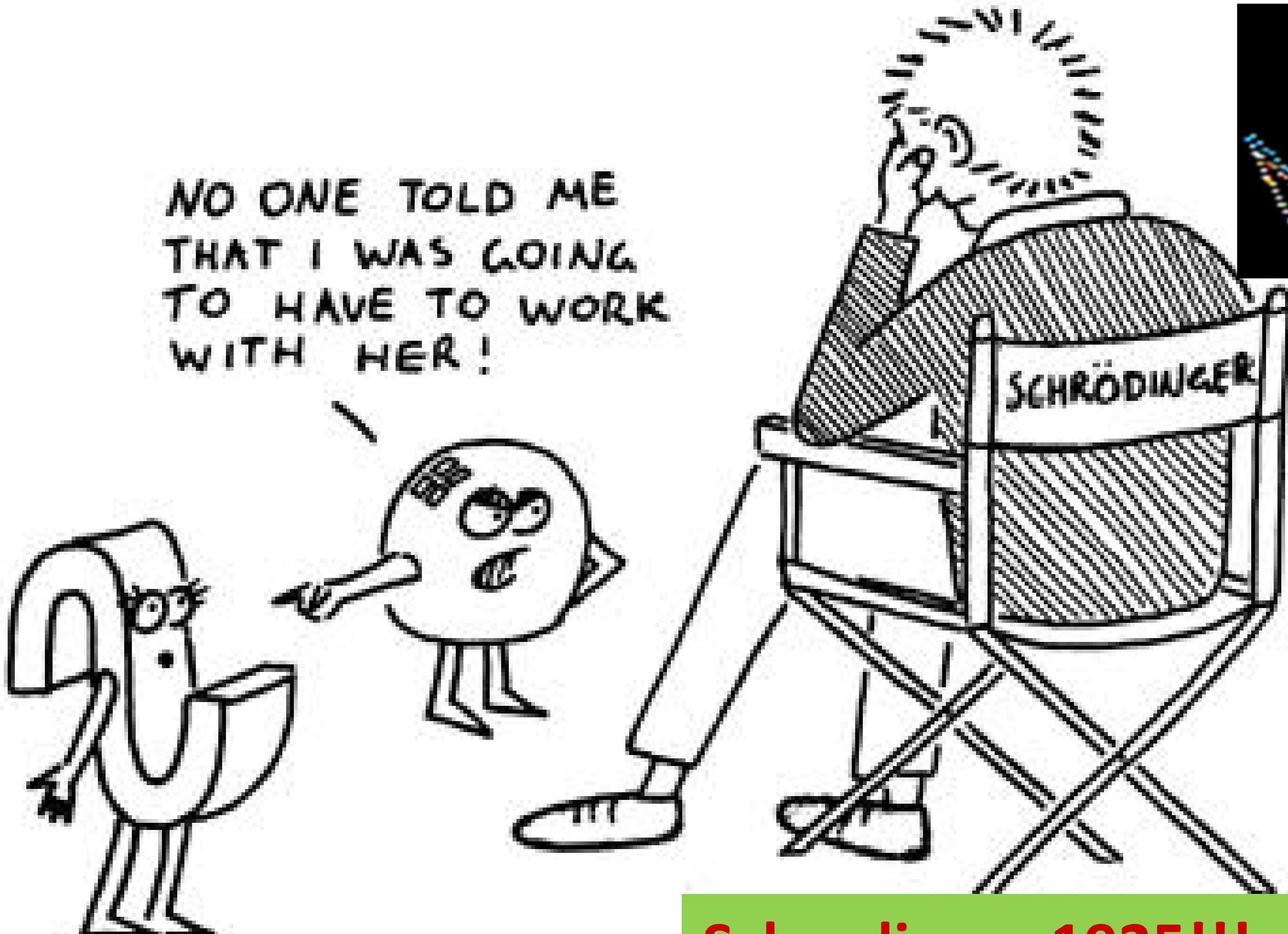
Richard Feynman on Quantum Behavior

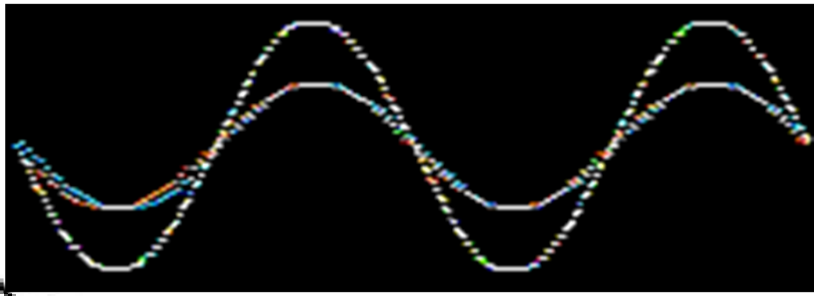
They behave in their own inimitable yet fascinating manner, which we call "Quantum Mechanical way"

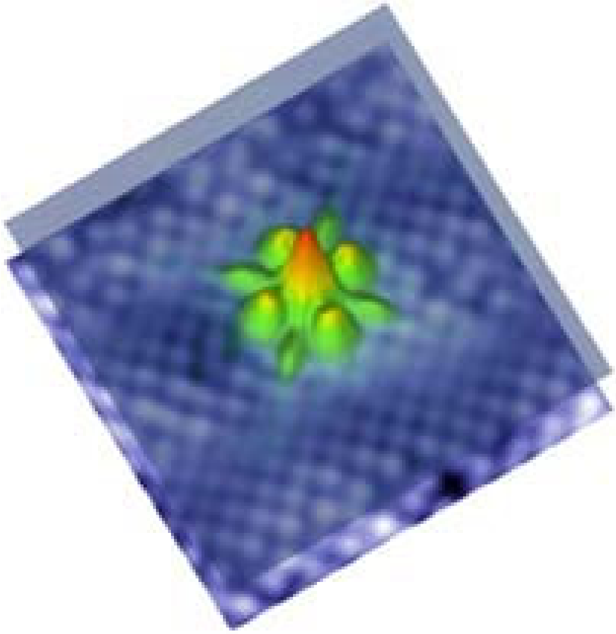
Best to be described mathematically!

Need a new theory for dynamics of electrons, atoms or molecules

- **Wavelike equation** for describing sub/atomic systems
- *Probabilistic*, **not deterministic** (non-newtonian)







Schrodinger 1925!!!

3-1 *The Schrödinger Equation Is the Equation for the Wave Function of a Particle*

We cannot derive the Schrödinger equation anymore than we can derive Newton's laws, and Newton's second law, $f = ma$, in particular. We shall regard the Schrödinger equation to be a fundamental postulate, or axiom of quantum mechanics, just as Newton's laws are fundamental postulates of classical mechanics. Even though we cannot derive the Schrödinger equation, we can at least show that it is plausible and perhaps even trace Schrödinger's original line of thought. We finished Chapter 1 with a discussion of matter

$$\boxed{H\Psi = E\Psi}$$

"We **CANNOT** derive Schrodinger equation anymore than we can derive Newton's laws"

$$\psi(x) = 2a\cos\left(\frac{2\pi x}{\lambda}\right)$$

$$\frac{d\psi(x)}{dx} = -2a\left(\frac{2\pi}{\lambda}\right)\sin\left(\frac{2\pi x}{\lambda}\right)$$

$$\frac{d^2\psi(x)}{dx^2} = -2a\left(\frac{2\pi}{\lambda}\right)^2\cos\left(\frac{2\pi x}{\lambda}\right)$$

$$= -\left(\frac{2\pi}{\lambda}\right)^2\psi(x)$$

$\lambda = \frac{h}{p}$

$E = K.E. + P.E.$

$= \frac{p^2}{2m} + V(x)$

$[E - V(x)]2m = p^2$

$$\frac{d^2\psi(x)}{dx^2} = -\left(\frac{p}{\hbar}\right)^2\psi(x)$$

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

$p^2 = 2m[E - V(x)]$

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}[E - V(x)]\psi(x)$$

3-1 *The Schrödinger Equation Is the Equation for the Wave Function of a Particle*

We cannot derive the Schrödinger equation anymore than we can derive Newton's laws, and Newton's second law, $f = ma$, in particular. We shall regard the Schrödinger equation to be a fundamental postulate, or axiom of quantum mechanics, just as Newton's laws are fundamental postulates of classical mechanics. Even though we cannot derive the Schrödinger equation, we can at least show that it is plausible and perhaps even trace Schrödinger's original line of thought. We finished Chapter 1 with a discussion of matter

$$\frac{\psi^2(x)}{dx^2} = -\frac{2m}{\hbar^2}[E - U(x)]\psi(x)$$

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

$$\underbrace{\left[\underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\text{K.E. operator}} + \underbrace{U(x)}_{\text{P.E. operator}}\right]}_{H}\psi(x) = E\psi(x)$$

$$\Downarrow$$

$$\hat{H}\psi(x) = E\psi(x)$$

$$\hat{H}\psi(x) = E\psi(x)$$

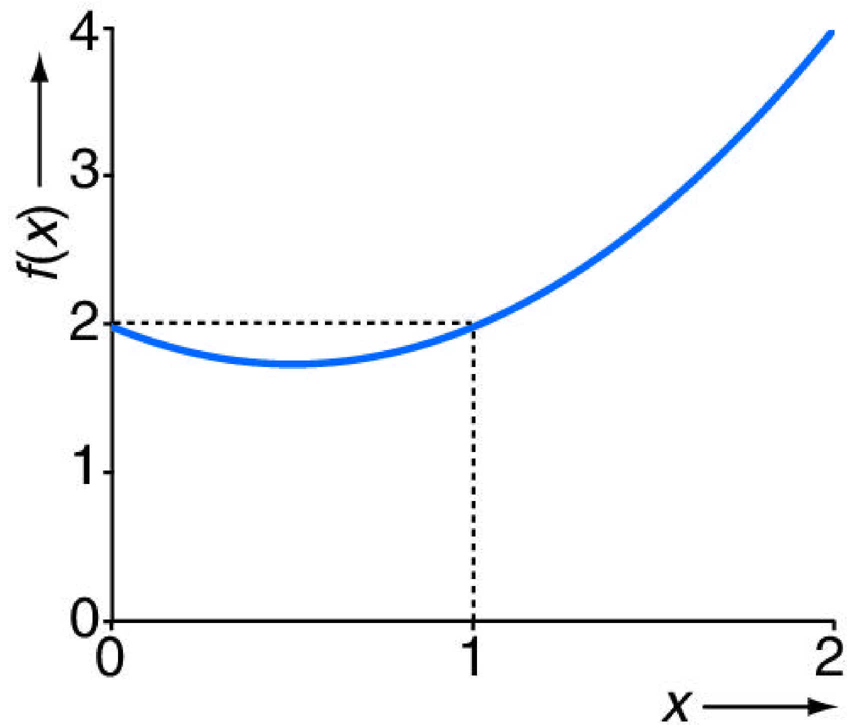
Wavefunction: Mathematical Function

In mathematics, a function is something which, for a given value of the appropriate variables, can be evaluated to give a number

Example: $x^2 - x + 2 = f(x)$

In quantum mechanics, the wave function is simply a mathematical function of relevant variable.

Example, for a single electron in the H atom, the wave function is a function of the coordinates x, y, and z which specify the position of the electron i.e. x, y and z are the variables



Wavefunction

- In quantum mechanics, wavefunction of a particle is a mathematical entity that contains all the dynamical information about the system.

- It contains where the particle can be found, its linear momentum, any property of the system that you ask about.

- It is the central carrier of information in quantum mechanics

Operator

$f(x) = \sin Ax$

operator

Operator is a mathematical object which acts on a function to give a new function

$\hat{H}\Psi = E\Psi$

$\frac{d}{dx} \sin Ax = +A \cos Ax$

$$x \; \underline{\sin(Ax)} = \underline{x \sin(Ax)}$$

operator | function | New function

"x" here is an operator for position

Operator for Energy: Hamiltonian

$\hat{H} \Rightarrow$ operator for energy

$$E_{tot} = T + V.$$

The operator for the kinetic energy along x-axis is

$$\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2},$$

The potential energy is a function of position $\hat{V} = V(x).$

Eigenfunctions and Eigenvalues

Eigenfunctions are a special set of functions which have the property that, when they are acted upon by a particular operator, they are unchanged, apart from being multiplied by a constant

The constant obtained is called eigenvalue

$$\hat{A}\phi = \lambda \times \phi.$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\phi(x) = \lambda\,\phi(x).$$

$$E_{\mathrm{tot}} = T + V.$$

$f(\theta) = \sin\theta$

$\frac{d}{d\theta}\sin\theta = 1\cos\theta$

$\frac{d^2}{d\theta^2}\boxed{\sin\theta} = -1\,\boxed{\sin\theta}$

eigen function

eigen value

Eigenfunctions and Eigenvalues

Eigenfunctions are a special set of functions which have the property that, when they are acted upon by a particular operator, they are unchanged, apart from being multiplied by a constant

The constant obtained is called eigenvalue

$$\hat{A}\,\phi = \lambda \times \phi.$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\phi(x) = \lambda\,\phi(x).$$

$$E_{\mathrm{tot}} = T + V.$$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}\phi(x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left[B\exp(Cx)\right] \\ &= CB\exp(Cx) \\ &= C\phi(x).\end{aligned}$$

Schrödinger equation of H-Atom: Cartesian Coordinates

$$\hat{H}\psi(x,y,z) = E.\psi(x,y,z)$$

Eigen Value

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + V(x, y, z)$$

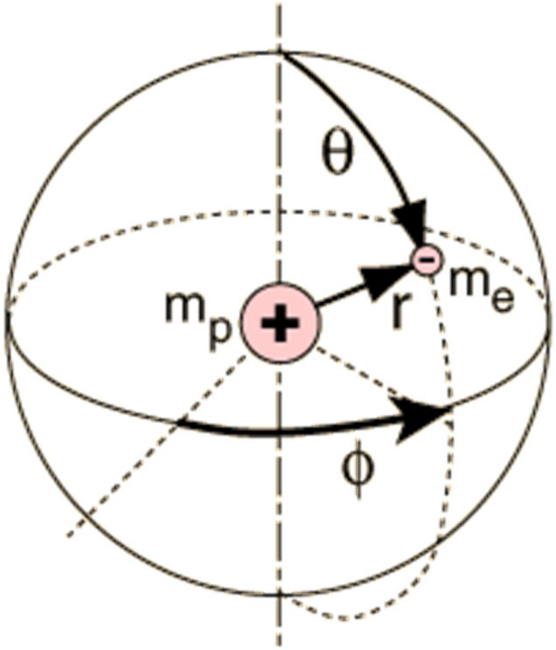
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) - \frac{e^2}{(x^2+y^2+z^2)^{1/2}}\psi(x,y,z) = E.\psi(x,y,z)$$

Road-Block: This 2nd order PDE with ***3 variables…***

Can not be separated!!!

Hamiltonian: Spherical Polar Coordinates

$$x = r\sin\theta\cos\phi$$
$$y = r\sin\theta\sin\phi$$
$$z = r\cos\theta$$



Solve this PDE →need to separate variables **r**, θ, ϕ: **POSSIBLE**

A Completely Solvable problem!!

(kind of rare, in QM!)