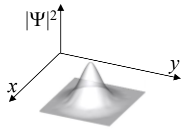
Schrödinger Equation

- Qauntum Mechanics is based on replacing particle trajectories in Newtonian mechanics with a time-varying state given by the **wave function** $\Psi(\vec{x},t)$
- Ψ interpreted as a probability amplitude for the particle being at location $\vec{x}=(x,y,z)$ at time t
  - specifically, probability of finding the particle in differential volume $dxdydz$ around $\vec{x}$ at time t

$$= \left|\Psi(\vec{x},t)\right|^2 dxdydz = \Psi\Psi^* dxdydz$$

complex conjugate



2-d representation

- Particle must be somewhere at time t, so constraint on Ψ is

$$\int\int\int_{-\infty}^{\infty} \Psi\Psi^* dxdydz = \int\int\int_{-\infty}^{\infty} \Psi\Psi^* dV = 1$$

- Also, Ψ must satisfy **Schrödinger Equation**

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{x},t)+V(\vec{x},t)\Psi(\vec{x},t)=i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t}$$

Laplacian Operator

$V(\vec{x},t)$ = ***Potential Energy*** *from field in which particle moving*

Schrödinger Equation: SOV Approach

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{x},t)+V(\vec{x},t)\Psi(\vec{x},t)=i\hbar\frac{\partial\Psi(\vec{x},t)}{\partial t}$$

- In many situations, $V=V(\vec{x})$; field is not time-dependent
- Then can apply separation of variables (SOV), and assume a solution of the form

$$\Psi(\vec{x},t)=\psi(\vec{x})\phi(t)$$

time-independent wave function

  - insert it into Schrödinger Eqn.

$$\frac{1}{\psi}\left[\frac{-\hbar^2}{2m}\nabla^2\psi+V\psi\right]=\frac{i\hbar}{\phi}\frac{d\phi}{dt}$$

  - two sides of eqn. are independent LHS=fn($\vec{x}$), RHS=fn(t)
    - so LHS = RHS = constant ≡ ***C***

Time-Independent Schrödinger Equation

- Thus we get 2 equations
- First examine time-dependence (RHS) $\frac{d\phi}{dt} = -i\frac{C}{\hbar}\phi$
  - solution of this ODE is $\phi(t) = Ae^{-i\frac{C}{\hbar}t}$
  - the parameter $C/\hbar$ is a frequency (e.g., s^{-1} units)
    - so our wave frequency is $\omega = C/\hbar$
    - but from photon analogy for particle/wave duality $\hbar\omega = \varepsilon \Rightarrow$ our constant $C = \varepsilon$
  - turns out A=1 to satisfy $\int\int\int_{-\infty}^{\infty} \psi\psi^* dV = 1$
- With C=ε on LHS, we get

$$\phi(t) = Ae^{-i\frac{\varepsilon}{\hbar}t}$$

(A → 1)

at any time, probability must =1 of particle being somewhere

time-independent Schrödinger Equation

$$\nabla^2\psi + \frac{2m}{\hbar^2}(\varepsilon - V)\psi = 0$$

solving this will provide information on quantized energies of our molelcules