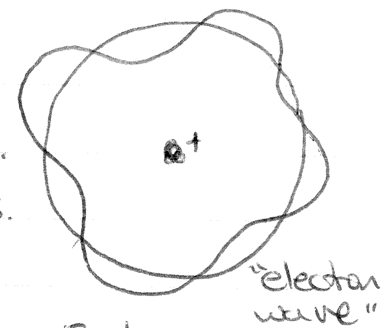
Schrödinger Equation

- Limitations of Bohr model:
  - only hydrogenic atoms, no molecules, crystals.
  - no fine structure or transition strengths.
  - orbits instead of waves & probability.



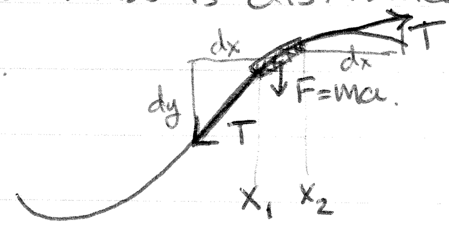
- deBroglie – hint at waves in the atom

$\Delta E = h\nu$ photon
$L = n\hbar$ electron.

- wave equation – describes propagation of waves.
  - differential equation, because mass is distributed.

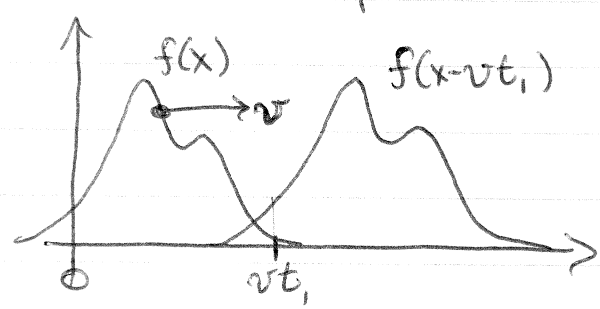
$$F_y = m \quad a_y$$

$$T\left(\frac{\partial y}{\partial x}\bigg|_2 - \frac{\partial y}{\partial x}\bigg|_1\right) = \rho\,\Delta x \cdot \frac{\partial^2 y}{\partial t^2}$$



$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{\rho}{T}\frac{\partial^2 y}{\partial t^2}}$$ wave equation for string.

- solution – dispersionless wave.



let $\boxed{y = f(x - vt)}$ v = constant = speed

$$\frac{\partial y}{\partial t} = f'(x-vt)\frac{\partial}{\partial t}(x-vt) = f' \cdot v$$

$$\frac{\partial^2 y}{\partial t^2} = -f'' \cdot v \cdot \frac{\partial}{\partial t}(x-vt) = f'' \cdot v^2$$

$$\frac{\partial^2 y}{\partial x^2} = f''(x-vt)$$

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$$

thus $v = \sqrt{\frac{T}{\rho}}$, velocity is a property of the medium.

- how do we apply this to matter waves where we don't know what the medium is?
  - a) use plane wave $\Psi = e^{i(kx - \omega t)}$.
  - b) require $E = \hbar\omega$, $p = \hbar k$, conservation of energy (dispersion relation) $E = \underbrace{\frac{p^2}{2m}}_{\text{kinetic}} + \underbrace{U(x)}_{\text{potential}}$

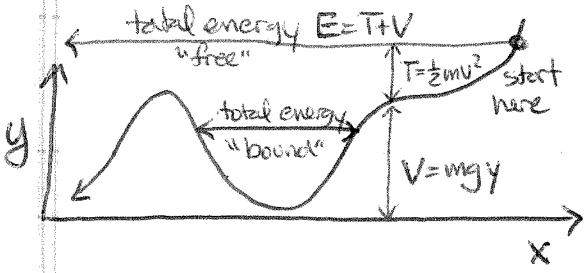
* "potential wells" $\vec{F} = -\nabla V \quad F_x = -\frac{\partial}{\partial x} V$

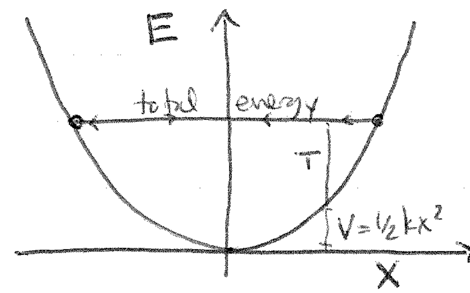
- gravity $\vec{F} = -mg\hat{y}$

  $V = mgy$

- harmonic oscillator $\vec{F} = -kx$

  $V = \frac{1}{2}kx^2$



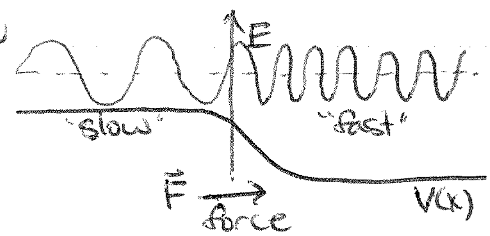


all states are bound.

* time dependent Schrödinger equation

$\frac{\partial}{\partial x} = ik \qquad \frac{\partial}{\partial t} = -i\omega$

(for plane waves).



$$\frac{\hbar^2 k^2}{2m} + V(x,t) = T + V = E = \hbar\omega$$

$$\boxed{\frac{-\hbar^2}{2m} \underbrace{\frac{\partial^2}{\partial x^2}}_{\nabla^2 \text{ in 3d.}} \Psi + V(x,t)\cdot\Psi = i\hbar\frac{\partial}{\partial t}\Psi}$$

"TDSE"

* time-independent Schrödinger equation.

if $\Psi(x,t) = e^{i(kx-\omega t)} = e^{ikx}\cdot e^{-i\omega t} \equiv \psi(x)\cdot\phi(t)$

- separation of variables.

$$\text{RHS} = i\hbar\frac{\partial}{\partial t}\psi(x)\cdot\phi(t) = \psi(x)\, i\hbar(-i\omega)e^{-i\omega t} = E\cdot\psi(x)\cdot\phi(t)$$

so: if $\Psi(x,t) = \psi(x)\cdot e^{-i\omega t}$

$$\boxed{\frac{-\hbar^2}{2m}\underbrace{\frac{\partial^2}{\partial x^2}}_{\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2} \text{ in 3 dimensions}}\psi(x) + V(x)\psi(x) = E\,\psi(x)}$$

"TISE"

total probability.

$$\boxed{|\psi|^2 = \psi^*\psi = 1}$$

normalization condition