Phys 5701   29 Sep 2020

Today: Schrödinger Wave Equation

$$\boxed{i\hbar \frac{\partial}{\partial t} \mathcal{U}(t) = H\,\mathcal{U}(t)}$$

where $\mathcal{U}(t)|\alpha, t=0\rangle = |\alpha, t\rangle$

Act on $|\alpha, t=0\rangle$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} |\alpha, t\rangle = H|\alpha, t\rangle$$

Position Representation: $\vec{X}|\vec{x}'\rangle = \vec{x}'|\vec{x}'\rangle$

$$\Rightarrow \boxed{i\hbar \frac{\partial}{\partial t} \langle \vec{x}'|\alpha, t\rangle = \langle \vec{x}'|H|\alpha, t\rangle}$$

write $\psi(\vec{x}', t) \equiv \langle \vec{x}'|\alpha, t\rangle$

"Wave Function"

For the time being...

$$H = \frac{1}{2m}\vec{p}^{\,2} + V(\vec{x})$$ "Particle of mass m"

$$\langle \vec{x}''| V(\vec{x}) |\vec{x}'\rangle = V(\vec{x}')\,\langle \vec{x}''|\vec{x}'\rangle$$
$$= V(\vec{x}')\,\delta^{(3)}(\vec{x}'-\vec{x}'')$$

Later: $\cdot\ V = V(\vec{x},t)$

$\cdot\ \langle \vec{x}'|V|\vec{x}''\rangle = v_1(\vec{x}')\,v_2(\vec{x}'')$

$\cdot\ V = \vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p} \qquad \vec{A} = \vec{A}(\vec{x},t)$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x}',t) = \langle \vec{x}'|\,\frac{\vec{p}^{\,2}}{2m}\,|\alpha,t\rangle$$
$$+ \underbrace{\langle \vec{x}'|\,V(\vec{x})\,|\alpha,t\rangle}_{= V(\vec{x}')\,\psi(\vec{x}',t)}$$

Recall: $\langle \vec{x}'|\vec{p}\,|\alpha,t\rangle = \frac{\hbar}{i}\vec{\nabla}'\langle \vec{x}'|\alpha,t\rangle$

so $\langle \vec{x}'|\vec{p}^{\,2}|\alpha,t\rangle = \langle \vec{x}'|\,\vec{p}\cdot\vec{p}\,|\alpha,t\rangle$
$$= \frac{\hbar}{i}\vec{\nabla}'\cdot\langle \vec{x}'|\vec{p}\,|\alpha,t\rangle$$
$$= -\hbar^2\,\vec{\nabla}'^2\,\psi(\vec{x}',t)$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{x}',t) = -\frac{\hbar^2}{2m}\vec{\nabla}'^2\psi(\vec{x}',t) + V(\vec{x}')\psi(\vec{x}',t)}$$

Partial Differential Equation

$\Rightarrow$ Solve it for $\psi(\vec{x}',t)$

Interpreting the Wave Function

Postulate: $|\langle a'|\alpha\rangle|^2$ = prob of measuring a' in $|\alpha\rangle$

$\Rightarrow$ $|\langle\vec{x}'|\alpha\rangle|^2 d^3x'$ = prob in $dV = d^3x'$

$$\Rightarrow \rho(\vec{x}',t) = |\langle\vec{x}'|\alpha,t\rangle|^2 = |\psi(\vec{x}',t)|^2$$

"Probability Density"

$$i\hbar\,\psi^* \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\psi^* \vec{\nabla}'^2\psi + \boxed{V}\,\psi^*\psi$$

$$-i\hbar\,\psi \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\psi \vec{\nabla}'^2\psi^* + \boxed{V}\,\psi^*\psi$$

$$\boxed{i\hbar\frac{\partial}{\partial t}(\underbrace{\psi^*\psi}_{\rho}) = -\frac{\hbar^2}{2m}\left[\psi^*\vec{\nabla}'^2\psi - \psi\vec{\nabla}'^2\psi^*\right]}$$

$$\begin{aligned}
&\psi^*\vec{\nabla}'^2\psi - \psi\vec{\nabla}'^2\psi^* \\
&= \psi^*\vec{\nabla}'^2\psi + \vec{\nabla}'\psi^*\cdot\vec{\nabla}'\psi - \vec{\nabla}'\psi^*\cdot\vec{\nabla}\psi - \psi\vec{\nabla}'^2\psi^* \\
&= \vec{\nabla}'\cdot\left[\psi^*\vec{\nabla}'\psi - \psi\vec{\nabla}'\psi^*\right]
\end{aligned}$$

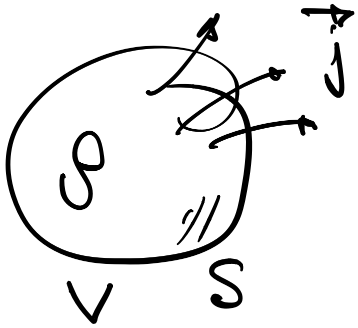
$$\Rightarrow \quad \frac{\partial\rho}{\partial t} = -\frac{\hbar}{2im}\vec{\nabla}'\cdot\left[\psi^*\vec{\nabla}'\psi - \psi\vec{\nabla}'\psi^*\right]$$

$$\equiv \vec{j}(\vec{x}',t)$$

$$\Rightarrow \quad \boxed{\frac{\partial}{\partial t}\rho(\vec{x}',t) + \vec{\nabla}'\cdot\vec{j}(\vec{x}',t) = 0}$$

CONTINUITY EQUATION

"Conservation Law"



If "stuff" is conserved,

$$\frac{d}{dt}\int_V \rho\, dV = -\oint_S \vec{j}\cdot d\vec{S}$$

$$= -\int_V \vec{\nabla}\cdot\vec{j}\, dV$$

or $\displaystyle\int\left[\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j}\right] dV = 0$

But V is arbitrary! $\Rightarrow$ $\displaystyle\frac{\partial\rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0$

But what is $\vec{j}$?

$$\vec{j}(\vec{x}',t) = \frac{\hbar}{2im}\left[\psi^*\vec{\nabla}'\psi - \psi\vec{\nabla}'\psi^*\right]$$

$$= \frac{\hbar}{m}\,\mathrm{Im}\left(\psi^*\vec{\nabla}'\psi\right)$$

$$\int_{\text{all space}} d^3x'\,\vec{j} = \frac{\hbar}{m}\,\mathrm{Im}\int d^3x'\,\psi^*\vec{\nabla}'\psi$$

$$= \frac{\hbar}{m}\,\mathrm{Im}\int d^3x'\,\langle\alpha,t|\vec{x}'\rangle\,\vec{\nabla}'\,\langle\vec{x}'|\alpha,t\rangle$$

$$= \frac{\hbar}{m}\,\mathrm{Im}\int d^3x'\,\langle\alpha,t|\vec{x}'\rangle\,\frac{i}{\hbar}\langle\vec{x}'|\vec{p}\,|\alpha,t\rangle$$

$$= \frac{1}{m}\underline{\int d^3x'}\,\langle\alpha,t|\underline{\vec{x}'\rangle\langle\vec{x}'|}\vec{p}\,|\alpha,t\rangle$$

i.e. $\int d^3x' \, \vec{j}(\vec{x}',t) = \frac{1}{m}\langle \vec{p}\rangle_t$

$= \text{"velocity"}$

"LOOKS LIKE A FLUID"

Time Independent Wave Equation

$|\alpha\rangle = |a'\rangle$ w/ $A|a'\rangle = a'|a'\rangle$ $[A,H]=0$

i.e. $|\alpha,t\rangle = \mathcal{U}(t)|\alpha\rangle$

$= e^{-iHt/\hbar}|a'\rangle$

But $H|a'\rangle = E_{a'}|a'\rangle$

$\psi(\vec{x}',t) = \langle \vec{x}'|\alpha,t\rangle$

$= e^{-iE_{a'}t/\hbar}\langle \vec{x}'|a'\rangle$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \vec{\nabla}'^2 \psi + V(\vec{x}')\psi$$

$$E_{a'} \langle \vec{x}' | a' \rangle = -\frac{\hbar^2}{2m} \vec{\nabla}'^2 \langle \vec{x}' | a' \rangle + V(\vec{x}') \langle \vec{x}' | a' \rangle$$

$$\equiv u_{a'}(\vec{x}')$$

$$= u_E(\vec{x}') = \langle \vec{x}' | E \rangle$$

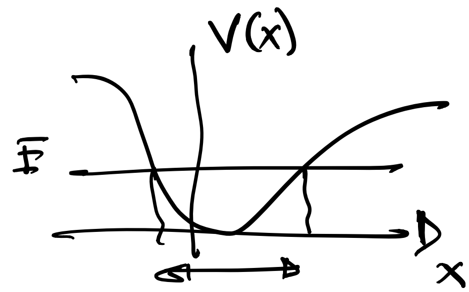
$$\boxed{-\frac{\hbar^2}{2m} \vec{\nabla}'^2 u_E + V(\vec{x}') u_E = E u_E(\vec{x}')}$$

"Time Indep Schrödinger Equation"

Solve for $u_E(\vec{x}')$ and eigenvalues E

Boundary Conditions

"Bound States" $\longrightarrow$



i.e. For $E < \lim_{|\vec{x}'| \to \infty} V(\vec{x}')$

$$\Rightarrow u_E(\vec{x}') \to 0 \quad \text{as} \quad |\vec{x}'| \to \infty$$

Free Particle i.e. $V=0$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2 u_E(\vec{x}) = E\,u_E(\vec{x})$$

write $E=\frac{\hbar^2}{2m}\vec{k}^2$ $\quad \vec{k}^2 = k_x^2+k_y^2+k_z^2$

and $u_E(\vec{x}) = u_x(x)\,u_y(y)\,u_z(z)$

"Separation of variables"

$$-\frac{d^2u_x}{dx^2}u_yu_z - \frac{d^2u_y}{dy^2}u_xu_z - \frac{d^2u_z}{dz^2}u_xu_y$$

$$= (k_x^2+k_y^2+k_z^2)\,u_xu_yu_z$$

$$\underbrace{\left[\frac{1}{u_x}\frac{d^2u_x}{dx^2}+k_x^2\right]}_{\text{Function } x} + \underbrace{\left[\frac{1}{u_y}\frac{d^2u_y}{dy^2}+k_y^2\right]}_{y} + \underbrace{\left[\frac{1}{u_z}\frac{d^2u_z}{dz^2}+k_z^2\right]}_{z} = 0$$

$=0 \qquad =0 \qquad =0$

$$\frac{d^2u_x}{dx^2} = -k_x^2 u_x \Rightarrow u_x(x) = C_x e^{ik_x x}$$

$$u_y(y) = C_y e^{ik_y y}$$

$$u_z(z) = C_z e^{ik_z z}$$

$$\Rightarrow u_E(\vec{x}) = C e^{i(k_x x + k_y y + k_z z)}$$

$$= C e^{i\vec{k}\cdot\vec{x}}$$

$$\psi(\vec{x},t) = C e^{i\vec{k}\cdot\vec{x}} e^{-iEt/\hbar}$$

$$= C e^{i(\vec{k}\cdot\vec{x} - \omega t)}$$

with $E = \underbrace{\frac{\hbar^2 \vec{k}^2}{2m} = \hbar\omega}$

$\boxed{\text{Plane Wave}}$

Dispersion Relation between $\vec{k}$ and ω

[i.e. $\vec{p} = \hbar\vec{k}$]