Lecture #18

Schrödinger picture: time-evolution of a state vector

Schrödinger equation: $i\hbar \frac{\partial}{\partial t}|\alpha, t_0; t\rangle = \hat{H}|\alpha, t_0, $

Typically you have to choose a basis to solve the Schrödinger equation $\Rightarrow$ in most cases x-representation is used (but not always, will discuss later)

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project on the x-basis

$\Downarrow$

$$i\hbar \frac{\partial}{\partial t} \underbrace{\langle \vec{x}' | \alpha, t_0; t\rangle}_{\Psi_\alpha(\vec{x}', t)} = \langle \vec{x}' | \hat{H} | \alpha, t_0; t\rangle$$

Consider Hamiltonian $\hat{H} = \frac{\hat{\vec{P}}^2}{2m} + \underbrace{\hat{V}(\vec{x})}_{\text{Hermitian operator}}$

$$\langle \vec{x}'' | \underbrace{\hat{V}(\vec{x})}_{\text{operator}} | \vec{x}' \rangle \overset{\text{locality condition}}{=} \underbrace{V(\vec{x}')}_{\substack{\text{function} \\ \text{not an operator}}} \underbrace{\delta^{(3)}(\vec{x}' - \vec{x}'')}_{\delta(x'-x'')\,\delta(y'-y'')\,\delta(z'-z'')}$$

$\vec{p}$ in $\vec{x}$-representation is $-i\hbar\vec{\nabla}$ $\Rightarrow$

$$\langle \vec{x}'|H|\alpha,t_0;t\rangle = \langle \vec{x}'|\frac{\hat{\vec{p}}^{\,2}}{2m}|\alpha,t_0;t\rangle +$$

$$+ \underbrace{\langle \vec{x}'|\hat{V}(\vec{x})|\alpha,t_0;t\rangle}_{= V(\vec{x}')\langle \vec{x}'|\alpha,t_0;t\rangle} = -\frac{\hbar^2}{2m}\underbrace{\vec{\nabla}'^{2}}_{=\Delta'}\langle \vec{x}'|\alpha,t_0;t\rangle + V(\vec{x}')\langle \vec{x}'|\alpha,t_0;t\rangle$$

$$\langle \vec{x}'|\frac{\hat{\vec{p}}^{\,2}}{2m}|\alpha,t_0;t\rangle = -\frac{\hbar^2}{2m}\overbrace{\Delta'}^{=\frac{\partial^2}{\partial x'^2}+\frac{\partial^2}{\partial y'^2}+\frac{\partial^2}{\partial z'^2}}\langle \vec{x}'|\alpha,t_0;t\rangle$$

recall Lecture #13 (eq. (13.3)) $\Rightarrow$ $\langle \vec{x}'|\hat{\vec{p}}|\alpha\rangle = -i\hbar\underbrace{\vec{\nabla}'}_{=\frac{\partial}{\partial \vec{x}'}}\langle \vec{x}'|\alpha\rangle$

So, the Schrödinger equation is:

$$i\hbar\frac{\partial}{\partial t}\langle \vec{x}'|\alpha,t_0;t\rangle = -\frac{\hbar^2}{2m}\Delta'\langle \vec{x}'|\alpha,t_0;t\rangle + V(\vec{x}')\langle \vec{x}'|\alpha,t_0;t\rangle \qquad (18.1)$$

Or, in more "familiar" terms, wave equation

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(\vec{x}',t) = -\frac{\hbar^2}{2m}\Delta'\psi_\alpha(\vec{x}',t) + V(\vec{x}')\psi_\alpha(\vec{x}',t)$$

What if at $t = t_0$ the system is in (3)
a stationary state $|\varphi_K\rangle$, i.e.

$$|\alpha, t_0\rangle = |\varphi_K\rangle$$

Then, $|\alpha, t_0; t\rangle = e^{-\frac{i}{\hbar}E_K t}|\alpha, t_0\rangle$

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Or, coming back to the x-basis and a wave function $\underset{\varphi_K}{\psi_\alpha}(\vec{x}', t) \Rightarrow$

$$\langle \vec{x}' | \varphi_K; t\rangle = \langle \vec{x}' | \varphi_K\rangle e^{-\frac{i}{\hbar}E_K t}$$

$\Downarrow$

substitute in Eq. (18.1)

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$$i\hbar \cdot \left(-\frac{i}{\hbar}E_K\right)\langle \vec{x}' | \varphi_K\rangle \cancel{e^{-\frac{i}{\hbar}E_K t}} = -\frac{\hbar^2}{2m} \cdot \Delta' \langle \vec{x}' | \varphi_K\rangle \cancel{e^{-\frac{i}{\hbar}E_K t}} + V(\vec{x}')\langle \vec{x}' | \varphi_K\rangle \cancel{e^{-\frac{i}{\hbar}E_K t}}$$

$\Downarrow$

$$-\frac{\hbar^2}{2m}\Delta' \overbrace{\langle \vec{x}' | \varphi_K\rangle}^{\text{energy eigenfunction } u_E(\vec{x}')} + V(\vec{x}')\langle \vec{x}' | \varphi_K\rangle = E_K \langle \vec{x}' | \varphi_K\rangle$$

time-independent wave equation

Can we do the same as we just did in x-representation for p-representation? ⇒ Sure! ⇒ how do we choose what's the best?

⇓

depends on the Hamiltonian

Consider $H = \frac{P^2}{2m} + V(x)$,

(in 1D for simplicity) $V(x) = \frac{1}{\cosh^2 x}$

Time-independent Schrödinger equation:

$$\underbrace{H u_E(x) = E u_E(x)}$$

$H|\varphi_k\rangle = E_k|\varphi_k\rangle$

or, in terms of the wave function in x-representation

⇓

$$\left(\underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}} + \frac{1}{\cosh^2 x}\right) u_E(x) = E u_E(x) \qquad (18.2)$$

need to present P in x-representation

What if we want to solve it in p-basis? ⇒ then need to present X in p-basis ⇒ (although can leave P as is)

$$\left[\frac{P^2}{2m} + \frac{1}{\cosh^2\left(i\hbar \frac{d}{dp}\right)}\right]\varphi_E(p) = E\varphi_E(p) \quad (18.3)$$

$\Downarrow$ $\uparrow$ X in p-representation

Brrrr!

$\Downarrow$

much easier to solve (18.2) than (18.3)

$\Downarrow$

for complicated $V(x) \Rightarrow$ better to use x-representation

Is there any physical situation for which p-representation is preferred? $\Rightarrow$

Consider a particle in a constant field f (e.g. electric field E_0, such as $f = eE_0$) $\Rightarrow$

$$H = \frac{P^2}{2m} - fX$$

X-basis: $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - fx\right)u_E(x) = Eu_E(x)$

p-basis: $\underbrace{\left(\frac{p^2}{2m} - f \cdot i\hbar\frac{d}{dp}\right)\varphi_E(p) = E\varphi_E(p)}$

simpler to solve since it is a 1st-order differential equation, while the x-basis one is a 2nd

What about a harmonic oscillator problem!?

$$H = \frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2$$ $\Rightarrow$ since both P and X are of the same power

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we will get similar 2^{nd} order differential equations in both X- and p- representation

$\Leftarrow$ Interestingly, this particular problem is ~~better~~ to solve in neither X- or P- basis $\Rightarrow$ we will talk about it next week!

Example: free particle in 1D $\Rightarrow$ $H = \frac{P^2}{2m}$

X-basis:
$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u_E(x) = E\,u_E(x)$$

$$\frac{d^2}{dx^2}u_E(x) + \underbrace{\frac{2mE}{\hbar^2}}_{=k^2}u_E(x) = 0$$

$$u_E(x) = C_1 e^{ikx} + C_2 e^{-ikx} \quad (18.4) \quad ; \quad E = \frac{\hbar^2 k^2}{2m}$$

P-basis:
$$\frac{P^2}{2m}\phi_E(p) = E\,\phi_E(p) \Rightarrow E = \frac{p^2}{2m}$$

$\Downarrow$

$$p = \pm\sqrt{2mE}$$

$$\Phi_E(p) = \tilde{C}_1 \, \delta(p - \sqrt{2mE}) + \tilde{C}_2 \, \delta(p + \sqrt{2mE})$$ ⑦

$\Downarrow$

Delocalised particle in the position space, but with well-defined momentum

Now let's go back to the position space and consider time evolution $\Rightarrow$

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} \quad (18.4a)$$

General approach ; separation of variables $\Rightarrow$

$$\Psi(x,t) = \tilde{\varphi}(x)\, T(t) \Rightarrow i\hbar \tilde{\varphi}(x) \underbrace{\frac{dT(t)}{dt}}_{= \dot{T}} = -\frac{\hbar^2}{2m} \underbrace{\frac{d^2\tilde{\varphi}}{dx^2}}_{= \tilde{\varphi}''} T(t)$$

$$\underbrace{\cancel{i\hbar}\frac{\dot{T}(t)}{T}}_{= \omega} = \underbrace{-\frac{\cancel{\hbar^2}}{2m} \frac{\tilde{\varphi}''(x)}{\tilde{\varphi}}}_{= \omega} \Rightarrow \dot{T}(t) + i\omega T(t) = 0$$

const

$\Downarrow$

$$T(t) = C e^{-i\omega t}$$

$$\tilde{\varphi}''(x) + \underbrace{\frac{2m\omega}{\hbar}}_{= k^2} \tilde{\varphi}(x) = 0$$

$$\omega = \frac{\hbar k^2}{2m}$$

$\Downarrow$

$$\tilde{\varphi}^{\#}(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$

$$\Psi(x,t) = \tilde{C}_1 e^{i(kx - \omega(k)t)} + \tilde{C}_2 e^{-i(kx + \omega(k)t)} \quad (18.5)$$

<u>Note:</u> We could have obtained Eq. (18.5) directly from (18.4) by propagating the stationary state $u_E(x)$ in time: $u_E(x) \cdot e^{-\frac{i}{\hbar}Et}$

$E = \frac{\hbar^2 k^2}{2m} = \hbar\omega(k)$

Is the wave function (18.5) well-behaved? $\Rightarrow$ not really! $\Rightarrow \int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx \to \infty \Rightarrow \Psi(x,t)$ is not square-integrable

Cannot represent a physical state?!!

Consider a <u>superposition</u> of plane waves given by (18.5) $\Rightarrow$ since all energies E (and the k's are allowed)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \varphi(p)\, \underbrace{e^{i(\overset{=p/\hbar}{k}x - \overset{=p/\hbar}{\omega(k)}t)}}_{u_E(x) e^{-\frac{i}{\hbar}Et}} dp \quad (18.6)$$

If the momentum of the particle is well-defined $\Rightarrow$

$p_0 = \hbar k_0$, $\omega(k_0) = \frac{\hbar k_0^2}{2m}$ $\Rightarrow$ then $\varphi_{E_0}(p) = \delta(p - p_0)$

$E_0 = \frac{p_0^2}{2m}$

So, $\Psi(x,t)$ given by 18.6 is a <u>1D wave-packet</u>. It satisfies (18.4a) and is square-integrable $\Rightarrow$ provides description of a free particle in 1D. (obviously, can be easily extended to 3D)