

Physics 570A

Lecture 8

Separation of space and time
in the Schrödinger equation

Often, $V = V(x)$, independent of time. Then one can write

$$\Psi(x, t) = \psi(x) \chi(t)$$

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

$$i\hbar \psi(x) \frac{\partial \chi(t)}{\partial t} = -\frac{\hbar^2}{2m} \chi(t) \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi \chi$$

$$\frac{i\hbar}{\chi(t)} \frac{\partial \chi}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi}{\partial x^2} + V(x)$$

R.H.S. depends only on x , L.H.S. 2

depends only on $t \Rightarrow$ both sides must be constants \circ

$$i\hbar \frac{\partial \chi}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi}{\partial x^2} + V(x) = E$$

$$\frac{\partial \chi}{\partial t} = -\frac{iE}{\hbar} \chi(t)$$

$$\chi(t) = \chi(0) e^{-\frac{iEt}{\hbar}}$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi(x) = E \psi(x)$$

time-independent Schrödinger equation (in 1D)

Each solution $\psi_n(x)$ of this 3
equation will correspond to a
particular value of the energy,

E_n :

$$\Psi_n(x, t) = \psi_n(x) e^{-i \frac{E_n t}{\hbar}}$$

These are called stationary
states or energy eigenstates.

It is clear from the correspondence
principle that E_n is the
energy of the system :

$$\psi_n^*(x) E_n \psi_n(x) = \psi_n^*(x) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_n(x)$$

$$E_n \int_{-\infty}^{\infty} dx |\psi_n|^2 = \int_{-\infty}^{\infty} dx \psi_n^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_n(x)$$

$$E_n = \langle T + V \rangle_n$$

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Q: Can E_n be complex?

$$\begin{aligned} \rho(x,t) &= \Psi^*(x,t) \Psi(x,t) \\ &= \psi^*(x) \psi(x) e^{-\frac{i(E_n - E_n^*)}{\hbar} t} \end{aligned}$$

Assuming conservation of particles,

$$0 = \frac{d}{dt} \int_{-\infty}^{\infty} \rho(x,t) dx = \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t} dx$$

$$= -\frac{i}{\hbar} (E_n - E_n^*) \int_{-\infty}^{\infty} |\psi(x)|^2 dx e^{-\frac{i(E_n - E_n^*)}{\hbar} t}$$

$\Rightarrow E_n = E_n^*$ for a closed system. Not only $\langle E \rangle$, but also the eigenenergies must be real.

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Q: What is the uncertainty ΔE in an eigenstate E_n ?

$$\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$$

$$= \sqrt{\langle \hat{H}^2 \rangle_n - E_n^2}$$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$\hat{H} \psi_n(x) = E_n \psi_n(x)$$

$$\hat{H}^2 \psi_n(x) = E_n^2 \psi_n(x)$$

$$\int_{-\infty}^{\infty} dx \psi_n^*(x) \hat{H}^2 \psi(x) = E_n^2 \int_{-\infty}^{\infty} dx |\psi_n(x)|^2$$

$$\langle \hat{H}^2 \rangle = E_n^2$$

$\Delta E = 0$. This is the

essential property of an energy eigenstate: it is a state of definite

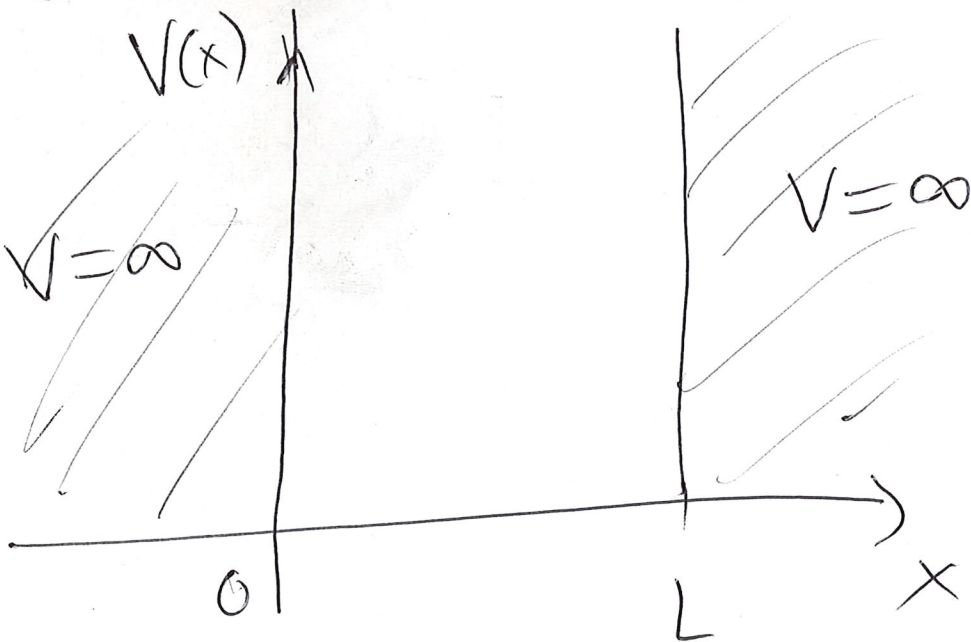
energy.

c.f. momentum eigenstates.

$$\psi(x,t) = \sum_n C_n \psi_n(x) e^{-iE_n t / \hbar}$$

Examples

i) particle in a box



$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi(x), \quad 0 < x < L \quad \boxed{7}$$

$$\psi(x) = 0, \quad x \leq 0 \quad \text{or} \quad x \geq L$$

$$\frac{d^2 \psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi(x) = -K^2 \psi(x)$$

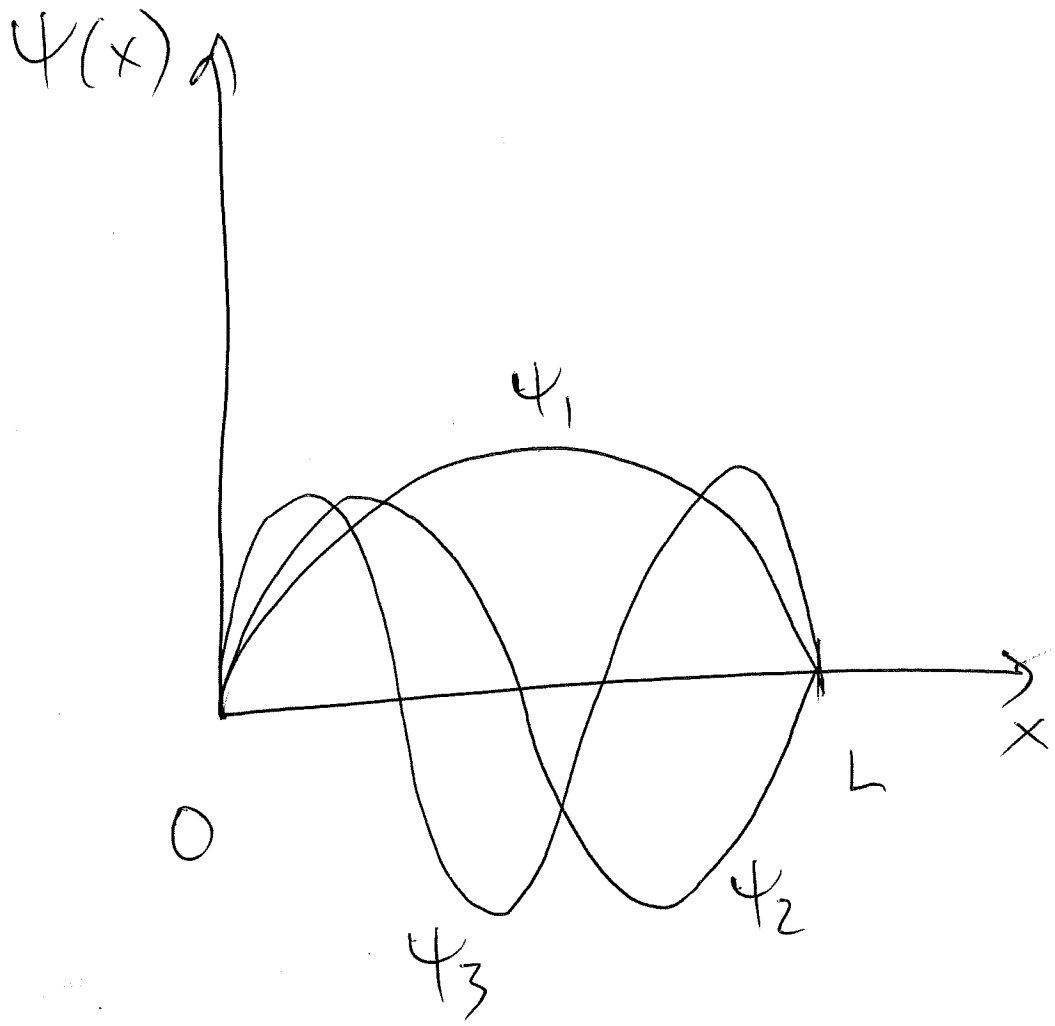
Define $\frac{2mE}{\hbar^2} = K^2$.

Solutions are:

$$\psi(x) = A \cos Kx + B \sin Kx$$

$$0 = \psi(0) = A$$

$$0 = \psi(L) = B \sin KL \Rightarrow K_n L = n\pi$$
$$n = 1, 2, 3, \dots$$



$$\psi_n(x) = B \sin\left(\frac{n\pi x}{L}\right)$$

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$$\int_0^L dx |\psi_n(x)|^2 = 1$$

$$B^2 \int_0^L dx \sin^2\left(\frac{n\pi x}{L}\right) = 1$$

$$B^2 \frac{L}{2} = 1$$

$$B = \sqrt{\frac{2}{L}}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2m L^2}$$

$$n = 1, 2, 3, \dots$$

Notice that

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$$\int_0^L dx \psi_n^*(x) \psi_{n'}(x) = \delta_{nn'}$$

We will see later that this is a general property of such eigenstates.

Quantum Beats

$$\Psi_n(x,t) = \psi_n(x) e^{-i \frac{E_n t}{\hbar}}$$

Consider

$$\phi(x) = a \psi_1(x) + b \psi_2(x)$$

is also

~~a soln of the time-independent~~

~~Schrödinger equation. What~~

is its time dependence?

$$\Phi(x,t) = a\psi_1(x)e^{-\frac{iE_1 t}{\hbar}} + b\psi_2(x)e^{-\frac{iE_2 t}{\hbar}} \quad \underline{10}$$

Proof :

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

$$E_1 a \psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + E_2 b \psi_2(x) e^{-\frac{iE_2 t}{\hbar}}$$

$$= a e^{-\frac{iE_1 t}{\hbar}} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_1(x)$$

$$+ b e^{-\frac{iE_2 t}{\hbar}} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi_2(x)$$

Q: What is $\rho(x,t) = |\Phi(x,t)|^2$?

$$\rho(x,t) = \left(a^* \psi_1(x) e^{\frac{iE_1 t}{\hbar}} + b^* \psi_2(x) e^{\frac{iE_2 t}{\hbar}} \right)$$

$$\times \left(a \psi_1(x) e^{-\frac{iE_1 t}{\hbar}} + b \psi_2(x) e^{-\frac{iE_2 t}{\hbar}} \right)$$

$$\begin{aligned}
 \rho(x,t) &= |a|^2 |\psi_1(x)|^2 + |b|^2 |\psi_2(x)|^2 \\
 &+ a^* b \psi_1(x) \psi_2(x) e^{i \frac{E_1 - E_2}{\hbar} t} \\
 &+ a b^* \psi_1(x) \psi_2(x) e^{-i \frac{E_1 - E_2}{\hbar} t}
 \end{aligned}$$

$$\text{Let } a = |a| e^{i\alpha}, \quad b = |b| e^{i\beta}$$

$$\begin{aligned}
 \rho(x,t) &= |a|^2 \psi_1^2(x) + |b|^2 \psi_2^2(x) \\
 &+ 2 |a| |b| \psi_1(x) \psi_2(x) \\
 &\quad \times \cos \left(\frac{E_1 - E_2}{\hbar} t + \beta - \alpha \right)
 \end{aligned}$$

The probability distribution oscillates at a frequency

$$\Omega_{12} = \frac{E_2 - E_1}{\hbar} \Rightarrow \text{gen. sol'n } \psi(x,t)$$

Wave-packet dynamics and scattering in 4D

Consider the wave packet

$$\Psi(x, t=0) = B e^{i k_0 x - \sigma_k^2 x^2}, \text{ which}$$

was discussed in lecture 4.

How does it evolve with time?

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \quad (\text{free particle})$$

$$\Psi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\Psi}(k, t) e^{ikx}$$

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \left[i\hbar \frac{\partial \tilde{\Psi}(k,t)}{\partial t} - \frac{\hbar^2 k^2}{2m} \tilde{\Psi}(k,t) \right] e^{ikx} = 0$$

$$\Rightarrow i\hbar \frac{\partial \tilde{\Psi}(k,t)}{\partial t} = \frac{\hbar^2 k^2}{2m} \tilde{\Psi}(k,t)$$

Solution:

$$\tilde{\Psi}(k,t) = \tilde{\Psi}(k, t=0) e^{-i\omega_k t}$$

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

$$\Psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{\Psi}(k, t=0) e^{i(kx - \omega_k t)}$$

$$= A \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx - i\omega_k t - \frac{(k-k_0)^2}{4\sigma_k^2}}$$

Let us expand

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$$\omega_k = \omega_0 + \left. \frac{d\omega}{dk} \right|_{k_0} (k - k_0) + \frac{1}{2} \left. \frac{d^2\omega}{dk^2} \right|_{k_0} (k - k_0)^2 + \dots$$

$$\omega_0 = \frac{\hbar k_0^2}{2m}$$

$$\left. \frac{d\omega}{dk} \right|_{k_0} = \frac{\hbar k_0}{m} = v_g$$

group velocity

= particle speed

$$\left. \frac{d^2\omega}{dk^2} \right|_{k_0} = \frac{\hbar}{m}$$

$$\omega_k \approx \omega_0 + v_g (k - k_0) + \frac{\hbar}{2m} (k - k_0)^2$$

$$\Psi(x, t) = A e^{i(k_0 x - \omega_0 t)} \int_{-\infty}^{\infty} \frac{dk}{2\pi}$$

$$\times e^{i(k - k_0)(x - v_g t) - a(k - k_0)^2}$$

$$a = \frac{1}{4\sigma_k^2} + \frac{i\hbar t}{2m}$$

Completing the square, and performing the Gaussian integral, one finds

$$\Psi(x,t) = C e^{i(k_0 x - \omega_0 t) - \frac{(x - v_g t)^2}{4a}}$$

Phase velocity $v_p = \frac{\omega_0}{k_0} = \frac{\hbar k_0}{2m} = \frac{1}{2} v_g$

$$|\Psi(x,t)|^2 = C^2 e^{-\frac{(x - v_g t)^2}{4a} - \frac{(x - v_g t)^2}{4a^*}}$$

$$= C^2 e^{-\frac{(x - v_g t)^2}{2\sigma_x(t)^2}}$$

→ probability wave packet moves at v_g

$$\sigma_x(t) = \frac{1}{2\sigma_k} \sqrt{1 + \left(\frac{2\hbar\sigma_k^2 t}{m}\right)^2}$$

For long times,

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$$\sigma_x(t) \approx \frac{\hbar \sigma_k}{m} t = \frac{\hbar \Delta k}{m} t = \Delta v t.$$

$$\Delta x \Delta p_x = \frac{\hbar}{2} \sqrt{1 + \left(\frac{2\hbar \sigma_k^2 t}{m}\right)^2} \geq \frac{\hbar}{2}$$

minimum-uncertainty wavepacket
spreads in coordinate space,
retains shape in momentum
space. Product of uncertainties
increases with time.