⑩ Important message about $\hat{p}$ conservation added.
⑦ Comment added on $\langle \hat{p}^2 \rangle$ and Δk

§ 2.4 Free Particle

$V = 0$ everywhere (or $V = \text{Const.}$)

This looks very simple, but is very subtle !!

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi \qquad E \geq 0,\ k \geq 0$$

(Can show $E<0 \rightarrow \psi$ diverges exponentially at $+\infty$ or $-\infty$ $\rightarrow$ not allowed.)

$$\psi = A e^{ikx} + B e^{-ikx}$$

What's so subtle about this?

These stationary states are NOT normalizable !

$$\int_{-\infty}^{\infty} dx\, \psi^*\psi = |A|^2\int_{-\infty}^{\infty} dx + |B|^2\int_{-\infty}^{\infty} dx + \underbrace{2|AB|\int_{-\infty}^{\infty} dx \cos(2kx+\varphi)}_{=0 \text{ if } k\neq 0}$$

$$\begin{cases} = (|A|^2+|B|^2)\cdot\infty & \text{if } k\neq 0 \\ = |A+B|^2\cdot\infty & \text{if } k=0 \ \Leftarrow \text{since } \psi = A+B \text{ if } k=0 \end{cases}$$

The pathology is that a free particle with a definite momentum $\hbar k$ has an absolutely uniform probability distribution in space !

What to do??? ---- Ask Mother Nature !

She might say, "My dear daughters and sons, your three pound gray wonder is such a phenomenon, and even its creation can exclaim 'infinity and beyond' --- but --- did you really think that the infinity, or the zero, is within the realm of your senses ?"

Indeed, one may say that ∞ and 0 in physics simply represent the limiting scales of a given experiment. This thought makes it plausible to consider following solutions for the non-normalizable free particle (plane wave) dilemma.

1. Consider instead a particle in a box (size L) or a particle on a circle (circumference L).
   Treat L as finite, but much much larger than any scale of a given problem.
   E.g., L ~ diameter of hair for an atomic problem.
   $\psi(x) = \frac{1}{\sqrt{L}} e^{\pm ikx}$ is a normalized solution!
   The only difference ⇒ k is quantized due to fixed boundary condition (particle in a box) or periodic boundary condition (particle on a circle).

2. We can never create or measure a plane wave that has an infinite extent, and that has a single wave vector. ⇒ Treat "wave packets" as physical, and treat "plane waves" as non-physical.
   i.e. $\Delta k = 0$

3. In a typical experiment, particle beams with sharply defined momentum are used. Use the plane wave solution as representing particle flux !!
   $\Delta p \approx 0$ but not zero

$$\psi(x) = A e^{ikx} \qquad j = \frac{1}{2m}\Big\{\psi^*\Big(-i\hbar\frac{\partial}{\partial x}\Big)\psi + \underbrace{c.c.}_{\text{Complex conjugate}}\Big\}$$

$$= \underbrace{|A|^2}_{\substack{\text{Interpret as \# of particles per}\\ \text{unit length (= volume)}}} \cdot \underbrace{\frac{\hbar k}{m}}_{\text{Velocity } \left(\frac{p}{m}\right)}$$

It is important to keep in mind all three of these solutions as they are all physical, some-what inter-related, and much used. The text emphasizes ②, which is fine. The major disadvantage of ② is that math is much harder, so the best strategy in the long run is to use ①, ③ but not forgetting that when physicists talk about plane waves they are always talking about narrow $(\Delta k \approx 0)$ wave packets!

Wave Packet

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \phi(k)\, e^{i\left(kx - \frac{\varepsilon(k)t}{\hbar}\right)}$$

$$\left(\varepsilon(k) = \frac{\hbar^2 k^2}{2m} \right)$$

$$\Psi(x,0) = \int_{-\infty}^{\infty} dk\, \phi(k)\, \frac{e^{ikx}}{\sqrt{2\pi}}$$

continuum analog of $\sum_n c_n \psi_n(x)$ ← somewhat different from book. consistent with Dirac.

How to get $\phi(k)$?

$$\phi(k) = \int_{-\infty}^{\infty} dx\, \Psi(x,0)\, \frac{e^{-ikx}}{\sqrt{2\pi}}$$

continuum analog of $c_n = \int dx\, \psi_n^* \Psi(x,0)$

Why? Plancherel's theorem of Fourier Transform.

Note that this math is most easily handled if one notes

$$\boxed{\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx}} \quad (2.144)$$

See math note

Properties of Stationary States in Free Space

$$\psi_k(x) \equiv \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad k \in \mathbb{R}$$

① Momentum eigenstate

$$\hat{p}\,\psi_k(x) = -i\hbar \frac{\partial}{\partial x}\psi_k = \underbrace{\hbar k}_{\text{momentum eigenvalue}}\,\psi_k(x)$$

(reflects the homogeneity of free space or the translational invariance of free space)

$\Rightarrow \frac{d}{dt}\langle \hat{p} \rangle = 0$ for <u>any</u> wave function $\Psi(x,t)$

② Orthogonality

Dirac δ function

$$\int_{-\infty}^{\infty} dx\, \psi_k^* \psi_{k'} = \delta(k-k')$$

$\Rightarrow$ continuum analog of $\int_{-\infty}^{\infty} dx\, \psi_n^* \psi_{n'} = \delta_{nn'}$

Kronecker δ Symbol

proof.) $$\int_{-\infty}^{\infty} dx\, \psi_k^* \psi_{k'} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k'-k)x} = \delta(k'-k) = \delta(k-k')$$

③ Completeness

Any function $f(x)$ can be written as

$$f(x) = \int_{-\infty}^{\infty} dk\, \tilde{f}(k)\, \psi_k(x)$$

In this case, this is just the Fourier theorem, and so the completeness can be <u>proven</u>. Like in the infinite well problem. However, generally, the completeness is not provable.

$$\tilde{f}(k) = \int_{-\infty}^{\infty} dx\, \psi_k^*(x)\, f(x) \quad \leftarrow \text{inverse Fourier Transform}$$

Properties of a wave packet

any wave packet

$$\Psi(x,t) = \int_{-\infty}^{\infty} dk\ \phi(k)\ \frac{e^{i(kx-\omega(k)t)}}{\sqrt{2\pi}}$$

$$\omega(k) = \begin{cases} \dfrac{\hbar k^2}{2m} & \text{for non-rel. free particle} \\ ck & \text{for light, sound wave} \\ \sqrt{gk\tanh(kD)} & \text{for water wave} \end{cases}$$

$\boxed{\omega(k) \text{ --- ``dispersion relation''}}$

Assume k is clustered near k_0 with small Δk.
[If not, $\Delta k \gg 1$, $\Rightarrow$ ΔE is large $\Rightarrow$ The wave packet deforms fast $\Rightarrow$ Wave packet description is not useful.]

I.e., we assume $\phi(k) \neq 0$ only when $k \approx k_0$.

Can set $\omega(k) \approx \omega_0 + \omega_0' \cdot (k-k_0)$

$$\omega_0' \equiv \left.\frac{d\omega}{dk}\right|_{k_0}$$

Define $s \equiv k - k_0$

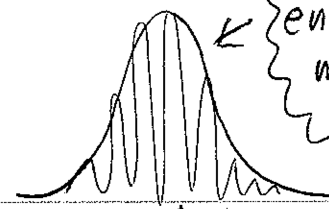
$$\Psi(x,t) \cong \int_{-\infty}^{\infty} ds\ \phi(k_0+s)\ \frac{e^{i[(k_0+s)x - \omega_0 t - \omega_0' s t]}}{\sqrt{2\pi}}$$

$$= \frac{e^{i(k_0 x - \omega_0 t)}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds\ \phi(k_0+s)\, e^{is(x-\omega_0' t)}$$

$$\left|\Psi(x,t)\right|^2 = \left| \int_{-\infty}^{\infty} ds\ \phi(k_0+s)\, e^{is(x-\omega_0' t)} \right|^2$$

$$= f(x - \omega_0' t)$$

Shape moving at the speed of ω_0'.
$\Rightarrow$ "group velocity"



envelope moves at v_g (important!!)

ripples move at v_p (not that important)

① Group velocity

$$v_g = \frac{d\omega}{dk}$$

[← different from the phase velocity

$$v_p = \frac{\omega}{k}$$]

For free particle ~~(non R)~~ energy $\frac{\hbar^2 k^2}{2m}$

$$v_g = \frac{\hbar k}{m}$$ ← matches expectation from classical mech.

Also, note that $j = \rho\, v_g$ for a plane wave.

② $\Psi(x,t)$ is normalizable as long as $\phi(k)$ is normalizable, in k space.

proof.) $$\int dx\, \Psi^* \Psi = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\, \phi^*(k')\phi(k) \times e^{i(k-k')x}$$

Using $\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, e^{i(k-k')x} = \delta(k-k')$, we get

$$\int_{-\infty}^{\infty} dx\, \Psi^* \Psi = \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk'\, \phi^*(k')\,\phi(k)\,\delta(k-k')$$

$$= \int_{-\infty}^{\infty} dk\, \phi^*(k)\,\phi(k) \qquad \text{QED}.$$

Not a coincidence

chap. 3 $\phi(k)$ = wave ftn in k space!

For instance, $\phi(k)$ can be defined as a gaussian function ⇒ $\Psi(x,t)$ is guaranteed to be normalizable. (It is actually a gaussian also.)

-7 ⊛ Note that if you calculate $\langle \hat{p}^2 \rangle$ for this wave function at any finite a $\rightarrow \langle \hat{p}^2 \rangle = \infty$ $\therefore \Delta k = \infty$, However if $a \to \infty$ $\langle \hat{p}^2 \rangle = 0$ $\therefore \Delta k = 0$

infinite energy! → Unphysical! and then

Source: Infinite slope of $\Psi(x,0)$ at $\pm a$.

Example 2.6

$$\Psi(x,0) = \begin{cases} A, & |x| \leq a \\ 0, & \text{otherwise} \end{cases}$$

$A > 0$,

$\Psi(x,t) = ?$

This problem is too idealized at $x = \pm a$. Should be taken as a limit of a smooth ftn.

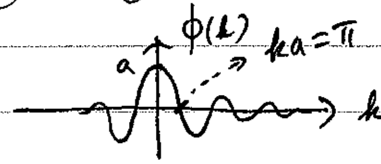
$A = \frac{1}{\sqrt{2a}}$ from normalization.

$$\phi(k) = \int_{-\infty}^{\infty} dx \, \frac{e^{-ikx}}{\sqrt{2\pi}} \Psi(x,0) = \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{\sqrt{2a}} \cdot \int_{-a}^{a} dx \, e^{-ikx}$$

$$= \frac{1}{\sqrt{\pi a}} \cdot \frac{\sin(ka)}{k}$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} dk \, \phi(k) \frac{e^{ikx}}{\sqrt{2\pi}} e^{-i\frac{\hbar k^2}{2m}t}$$

$$= \frac{1}{\pi\sqrt{2a}} \cdot \int_{-\infty}^{\infty} dk \, \frac{\sin(ka)}{k} e^{ikx} e^{-i\frac{\hbar k^2}{2m}t}$$



⊛ **General properties**

The k-width of $\phi(k) \sim \frac{1}{a}$

$\Delta x \sim a \qquad \Delta k \sim \frac{1}{a} \quad \Rightarrow \Delta x \cdot \Delta k \sim 1$

Uncertainty Principle !!

Extreme Case

① $a \to 0 \quad \Rightarrow \quad \sin(ka) \approx ka \qquad \phi(k) \approx \sqrt{\frac{a}{\pi}}$

(for $k \ll \frac{1}{a}$)

Δx small $\qquad\qquad \Delta k$ large

② $a \to \infty \quad \Rightarrow \quad \phi(k) = \sqrt{\frac{a}{\pi}} \cdot \frac{\sin(ka)}{ka} \sim O\left(\frac{1}{\sqrt{a}}\right)$ if $ka \gg 1$

$\sim O(\sqrt{a})$ if $ka \ll 1$

$\therefore \phi(k)$ is (localized / peaked) within $\sim \frac{1}{a}$

Prob. 2.22 Gaussian Wave Packet

$$\Psi(x,0) = A e^{-ax^2} \qquad A, a \in \mathbb{R},\ a>0$$

(a) Normalize ⋯ $A = ?$ $\quad \int dx\, |\Psi|^2 = 1$

$$\Rightarrow A^2 \cdot \int dx\, e^{-2ax^2} = A^2 \cdot \frac{1}{\sqrt{2a}} \cdot \sqrt{\pi} = 1 \Rightarrow A = \sqrt[4]{\frac{2a}{\pi}}$$

(b) $\Psi(x,t) = ?$

$$\boxed{\int_{-\infty}^{\infty} dx\, e^{-(ax^2+bx)} = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}}} \quad (\ast)$$

math note M3

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\, \phi(k)\, e^{i(kx - \frac{\hbar k^2}{2m}t)}$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int dx\, \Psi(x,0)\, e^{-ikx}$$

$$= \frac{1}{\sqrt{2\pi}} A \int_{-\infty}^{\infty} dx\, e^{-(ax^2+ikx)} \overset{(\ast)}{=} \frac{A}{\sqrt{2a}} \cdot e^{-\frac{k^2}{4a}}$$

$$\Psi(x,t) = \frac{A}{2\sqrt{\pi a}} \int dk\, e^{-\left[\left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)k^2 - ixk\right]}$$

$$\overset{(\ast)}{=} \frac{A}{2\sqrt{\pi a}} \cdot \frac{\sqrt{\pi}}{\sqrt{\frac{1}{4a} + \frac{i\hbar t}{2m}}} \cdot \exp\left[\frac{-x^2}{4 \cdot \left(\frac{1}{4a} + \frac{i\hbar t}{2m}\right)}\right]$$

$$= A \cdot \frac{1}{\sqrt{1 + i\frac{2a\hbar t}{m}}} \cdot \exp\left[-\frac{ax^2}{1 + i\frac{2a\hbar t}{m}}\right]$$

$$A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}$$

$$w \equiv \sqrt{\frac{a}{1 + \left(\frac{2a\hbar t}{m}\right)^2}}$$

(c) $|\Psi(x,t)|^2 = ?$

$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}} \cdot \frac{1}{\sqrt{1 + \left(\frac{2a\hbar t}{m}\right)^2}} \cdot \exp\left[-\frac{2ax^2}{1 + \left(\frac{2a\hbar t}{m}\right)^2}\right]$$

$$= \sqrt{\frac{2}{\pi}} \cdot w \cdot \exp\left[-2w^2x^2\right] \Leftarrow \text{gaussian with } \sigma = \frac{1}{2w}$$

$$\frac{1}{2\sigma^2} = 2a \qquad \boxed{\sigma = \frac{1}{2\sqrt{a}}}$$

$$\frac{1}{\sqrt{2\pi}\,\sigma} = \sqrt{\frac{2}{\pi}}\sqrt{a}$$

Check → ok.

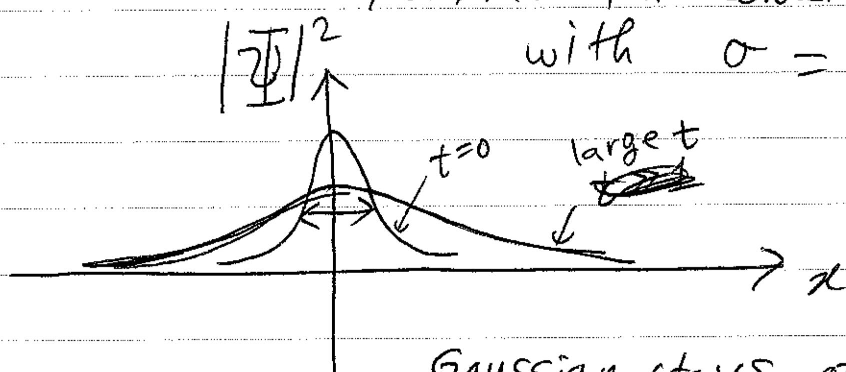
At $t=0$, $\omega = \sqrt{a}$

$$|\Psi(x,0)|^2 = \sqrt{\frac{2}{\pi}}\sqrt{a}\cdot e^{-2ax^2}$$

Gaussian ftn with $\sigma = \frac{1}{2\sqrt{a}}$ centered at 0.

At $t \to$ large, e.g. $\frac{2a\hbar t}{m} \gg 1 \Rightarrow \omega \simeq \sqrt{a}\cdot\frac{m}{2a\hbar t}$

→ Gaussian ftn centered at 0 with $\sigma = \cancel{\frac{1}{2}}\cdot\frac{\cancel{2}a\hbar t}{m\sqrt{a}} = \frac{\sqrt{a}\,\hbar t}{m}$



Gaussian stays at $X=0$
- broadens as $t\uparrow$
- height ↓ accordingly

Total area → conserved.
(~ width × height)

(d) $\langle x\rangle = 0 \quad \langle p\rangle = 0$

$\langle x^2\rangle = \frac{1}{4\omega^2} \quad \sigma_x = \frac{1}{2\omega}$

$\langle p^2\rangle = ?$ Need to take $-\hbar^2\frac{\partial^2\Psi}{\partial x^2}$

$$\Psi(x,t) = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}}\cdot\frac{1}{\sqrt{Z}}\cdot e^{-\frac{ax^2}{Z}} \qquad Z \equiv 1 + i\frac{2a\hbar t}{m}$$

$$\langle p^2\rangle = \sqrt{\frac{2a}{\pi}}\cdot\frac{1}{\sqrt{zz^*}}\cdot\int dx\, e^{-\frac{ax^2}{z^*}}(-\hbar^2)\boxed{\frac{\partial^2}{\partial x^2}e^{-\frac{ax^2}{z}}}$$

$$\frac{\partial^2 e^{-\frac{ax^2}{z}}}{\partial x^2} = \frac{\partial}{\partial x}\left[-\frac{2ax}{z}e^{-\frac{ax^2}{z}}\right] = -\left(\frac{2a}{z}-\left(\frac{2ax}{z}\right)^2\right)e^{-\frac{ax^2}{z}}$$

$$\therefore \langle p^2\rangle = \sqrt{\frac{2a}{\pi}}\cdot\frac{\hbar^2}{\sqrt{zz^*}}\frac{2a}{z}\underbrace{\int dx\left(1-\frac{2ax^2}{z}\right)e^{-\frac{2ax^2}{zz^*}}}_{\sqrt{\frac{zz^*}{2a}}\sqrt{\pi}-\frac{2a}{z}\sqrt{\left(\frac{zz^*}{2a}\right)^3}\cdot\frac{1}{2}\cdot\sqrt{\pi}}$$

$$= \frac{2a\hbar^2}{z}\cdot\left[1-\frac{\cancel{2a}}{\cancel{z}}\frac{\cancel{z}z^*}{\cancel{2a}}\cdot\frac{1}{2}\right]$$

$$1-\frac{z^*}{2} = 1-\frac{1}{2}\left(1-i\frac{2a\hbar t}{m}\right) = \frac{1}{2}+i\frac{a\hbar t}{m} = \frac{1}{2}z$$

$$= a\hbar^2 \ (!)$$

$$\therefore \sigma_p = \sqrt{a}\,\hbar$$

Why $\frac{d}{dt}\langle\hat{p}^2\rangle = \frac{d}{dt}\langle\hat{p}\rangle = 0$?
Translational invariance
$\Rightarrow$ $\hat{p}$ is conserved.
In QM, it means

$\frac{d}{dt}\langle\hat{p}\rangle = 0$
$\frac{d}{dt}\langle f(\hat{p})\rangle = 0$

for any $\Psi(x,t)$ and $f(\hat{p})$
BUT only in free space with $V=0$ or const.

(e) $$\sigma_x\sigma_p = \frac{1}{2w}\cdot\sqrt{a}\,\hbar$$

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

$$w \le \sqrt{a} \quad (= \text{ at } t=0)$$

$$\sigma_x\sigma_p \ge \frac{\hbar}{2}$$

minimum uncertainty at $t=0$

σ_p : fixed, $\sigma_x \uparrow$ as $t\uparrow$