LL 13/10/2010

Quantum ("wave") Mechanics

Postulates (simple, one-particle version)

"Statics"

(1) complex wave function $\psi(x,y,z;t)$
contains all available information on the system

(2) ψ, $\vec{\nabla}\psi$: finite, continuous, single-valued
for all accessible values of x, y, z, t

(3) $\underbrace{\psi^*\psi}_{|\psi|^2} \, dV$: probability to find the particle in dV

$dV = dx\,dy\,dz$

(4) dynamical variable $\alpha \implies$ "operator" $\hat{\alpha}$ (*)
expectation value $\langle\alpha\rangle = \int_V \psi^* \hat{\alpha} \psi \, dV$

"Dynamics"

(5) $\psi(x,y,z,t)$: solution of the "wave equation" (Schrödinger)

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + U(x,y,z,\dots)\psi$$

i : imaginary unit.

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ "Laplacian operator"

(*) "Correspondence principle" ...

result : $x, y, z \xrightarrow{\text{operators}} x, y, z$

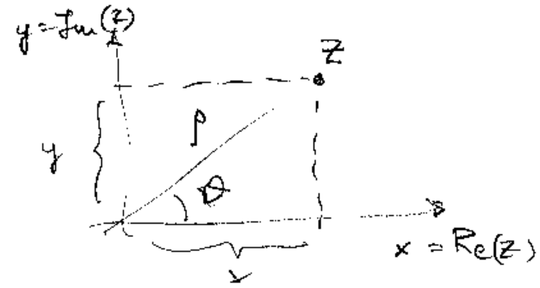
$p_x, p_y, p_z \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x}, \frac{\hbar}{i}\frac{\partial}{\partial y}, \frac{\hbar}{i}\frac{\partial}{\partial z}$

$$\begin{cases} \langle x\rangle = \int_V \psi^* x \psi \, dV \\ \langle p_x\rangle = \int_V \psi^* \frac{\hbar}{i}\frac{\partial\psi}{\partial x} \, dV \end{cases}$$

Reminder: complex numbers

$i = \sqrt{-1}$ $\quad i^2 = -1$ $\quad$ imaginary unit.

$$\begin{cases} z = x + iy \\ \quad \text{"real part"} \uparrow x, \quad \text{"imaginary part"} \uparrow y \end{cases}$$



complex conjugate

$z^* = x - iy$

modulus

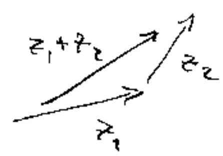
$$|z|^2 = z^* z = x^2 + y^2 = \rho^2 \qquad \rho = \sqrt{|z|^2} = \sqrt{x^2 + y^2}$$

phase

$$\theta = \operatorname{atan} \frac{y}{x}$$

$$z = x + iy = \rho e^{i\theta} = \rho(\cos\theta + i \operatorname{sen}\theta) \qquad \begin{aligned} x &= \rho\cos\theta \\ y &= \rho\sin\theta \end{aligned}$$

<u>Sum</u> $\quad z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2)$



<u>product</u> $\quad z_1 \cdot z_2 = \rho_1 \rho_2 \, e^{i(\theta_1 + \theta_2)}$

<u>ratio</u> $\quad \dfrac{z_1}{z_2} = \dfrac{\rho_1}{\rho_2} \, e^{i(\theta_1 - \theta_2)}$

NB. extension real functions $\longrightarrow$ complex functions

$$f(z) = u(x,y) + i v(x,y)$$

$$e^z \equiv 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots \qquad \text{with } z \text{ a complex number!}$$

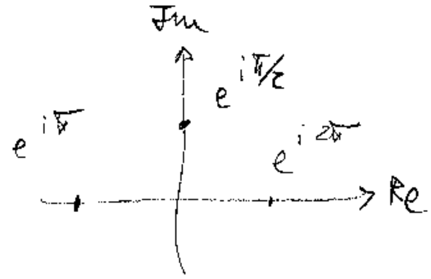
$$e^{z_1} e^{z_2} = e^{z_1 + z_2}$$

in particular: if z pure imaginary:

$$e^{i\phi} = 1 + (i\phi) + \frac{(i\phi)^2}{2!} + \frac{(i\phi)^3}{3!} = \begin{cases} \overbrace{1 - \frac{\phi^2}{2!} + \frac{\phi^4}{4!} - \dots}^{\cos\phi} \\ + i \underbrace{\left(\phi - \frac{\phi^3}{3!} + \frac{\phi^5}{5!} - \dots\right)}_{\sin\phi} \end{cases}$$

$$\overset{!}{=} \cos\phi + i \operatorname{sen}\phi$$

exercise: (complex numbers)



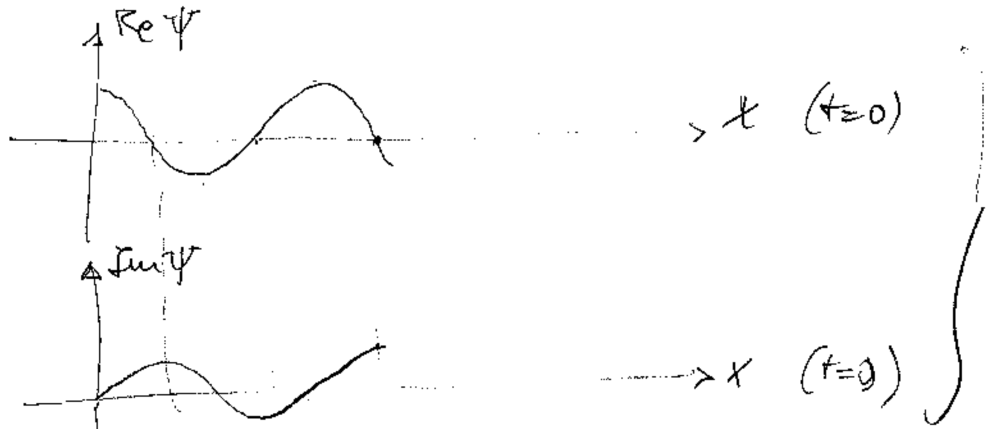
$$\begin{cases} e^{i\pi} = ? \quad -1 \\ e^{-i\pi} = ? \quad -1 \\ e^{i\pi/2} = ? \quad i \\ e^{in\pi} = ? \quad (-1)^n \quad n \text{ integer} \end{cases}$$

and: $\sin z = \dfrac{e^{iz} - e^{-iz}}{2i}$; $\cos z = \dfrac{e^{iz} + e^{-iz}}{2}$

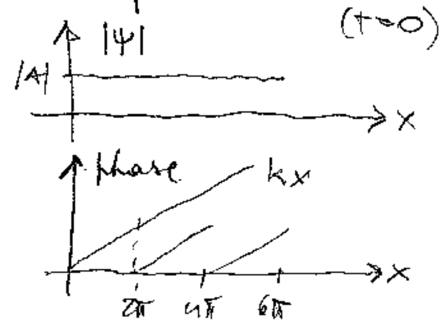
Application to waves

$$A e^{i(kx - \omega t)} = A\Big[\underbrace{\cos(kx-\omega t)}_{Re} + i \underbrace{\sin(kx-\omega t)}_{Im}\Big] = \Psi(x,t)$$

represents a travelling wave, with $(t=0)$



or, equivalent representation: (t=0)



- in classical e.m. waves, (or circuits ...) the use of complex numbers is only a matter of convenience: the algebra is simpler, but at the end the observable quantities correspond to the real part.

- In quantum mechanics, wave functions are inherently complex !!

Fourier series and Fourier transforms.

from: M.L. Boas, Mathematical methods in the physical sciences, J. Wiley & Sons, ch. 7 (p. 297 - 334); Ch. 15 (p. 647 - 662)

[A DIGRESSION ON MATHEMATICS]

Motivation, examples:

① - see discussion of (transverse) mechanical waves on a string with fixed ends at $x=0$ and $x=L$.

② - see applets (moodle site and on the internet)
$\Rightarrow$ get a qualitative feeling for what we are talking about.

③ - applications
- sound,
- electrical circuits,
- etc...

④ other useful expansions in series: power, etc.

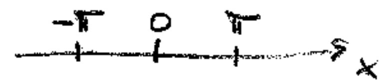
Outline:

① "Fourier coefficients" and "Dirichlet conditions" for (periodic) functions on the interval $[-\pi, \pi]$; Complex form of Fourier series.

② other intervals: for example $[0, 2\pi]$, $[-\ell, \ell]$, $[0, 2\ell]$, ... L
[Parseval's theorem?]

③ "Fourier transforms"
[Parseval's theorem?]

1. Fourier coefficients

to simplify notations : interval $[-\pi, \pi]$ 

expand a given $f(x)$, with period 2π,$^{(*)}$ in a series of :

$$\left.\begin{array}{l}\sin mx \\ \cos mx\end{array}\right\} m = 1, 2, \ldots \qquad \text{(all have period } 2\pi\text{)}$$

Def. "Fourier series" :

$$f(x) \underset{(?)}{=} \frac{1}{2} a_0 + a_1 \cos x + a_2 \cos 2x + \ldots$$
$$+ b_1 \sin x + b_2 \sin 2x + \quad =$$

$$= \frac{1}{2} a_0 + \sum_{1}^{\infty} {}_n\, a_n \cos nx + \sum_{1}^{\infty} {}_n\, b_n \cos nx$$

one can prove that (see M.L.Boas) : "orthonormality conditions" :

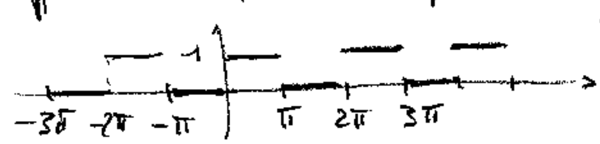
$$\begin{cases} \frac{1}{2\pi} \int_{-\pi}^{\pi} \sin mx \cos nx \, dx = 0 \\ \frac{1}{2\pi} \int_{-\pi}^{\pi} \sin mx \sin nx \, dx = \frac{1}{2} \delta_{mn} = \begin{cases} 0 & m \neq n \\ \frac{1}{2} & m = n \end{cases} \\ \frac{1}{2\pi} \int_{-\pi}^{\pi} \cos mx \cos nx \, dx = \frac{1}{2} \delta_{mn} = \begin{cases} 0 & m \neq n \\ \frac{1}{2} & m = n \end{cases} \end{cases}$$

and that the "Fourier coefficients" (constants!) are given by :

$$\begin{cases} a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx \, dx & \left(a_0 = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \, dx \right) \\ b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx \, dx & \text{(proof : see M.L. Boas)} \end{cases}$$

Exercise : find the Fourier coefficients for a "square wave" voltage

$$f(x) = \begin{cases} 0 & -\pi < x < 0 \\ 1 & 0 < x < \pi \end{cases}$$



Solution : $f(x) = \frac{1}{2} + \frac{2}{\pi} \left(\frac{\sin x}{1} + \frac{\sin 3x}{3} + \frac{\sin 5x}{5} + \ldots \right)$

2. Dirichlet conditions

$$f(x)\begin{cases}\text{period } 2\pi \\ \text{single-valued in } [-\pi,\pi] \\ \text{finite number of minima and maxima in } [\pi,\pi] \\ \text{finite } \int_{-\pi}^{\pi}|f(x)|\,dx \\ \text{finite number of discontinuities in } [\pi,\pi]\end{cases} \Longrightarrow$$

The Fourier series converges to $f(x)$ for all the points where $f(x)$ is continuous; at jumps it converges to the mid point of the jump.

(counter-examples for functions not satisfying these conditions)

3. Complex form of Fourier Series

Using complex numbers, the notation becomes more compact and easy to remember:

$$\sin nx = \frac{e^{inx}-e^{-inx}}{2i} \qquad \cos nx = \frac{e^{inx}+e^{-inx}}{2}$$

$$f(x) = \frac{1}{2}a_0 + a_1\frac{e^{ix}+e^{-ix}}{2} + a_2\frac{e^{i2x}+e^{-i\cdot 2x}}{2} + \dots$$
$$+ b_1\frac{e^{ix}-e^{-ix}}{2i} + b_2\frac{e^{i2x}-e^{-i2x}}{2i} + \dots$$

$$= \underbrace{\frac{1}{2}a_0}_{c_0} + \overbrace{\frac{1}{2}(a_1-ib_1)}^{c_1}e^{ix} + \overbrace{\frac{1}{2}(a_2-ib_2)}^{c_2}e^{i2x} + \dots$$
$$+ \underbrace{\frac{1}{2}(a_1+ib_1)}_{c_{-1}}e^{-ix} + \underbrace{\frac{1}{2}(a_2+ib_2)}_{c_{-2}}e^{-i2} + \dots$$

$$= \sum_{-\infty}^{-\infty}{}_n\, c_n e^{inx}$$

and, in this case, with $f(x)$ real:

$$c_{-n} = c_n^*$$

Complex Fourier series - cont.

But: there should be a way to find the c_n coefficients directly:

$$\boxed{f(x) = \sum_{n=-\infty}^{n=+\infty} c_n e^{inx}} \qquad x \in [-\pi, \pi]$$

$\uparrow$ $c_n = ?$

Relatively easy to check that the correct recipe is:

$$\frac{1}{2\pi}\int_{-\pi}^{+\pi} f(x)\, e^{-imx}\, dx = \sum_{-\infty}^{+\infty}{}_{n} \frac{1}{2\pi} c_n \underbrace{\int_{-\pi}^{+\pi} \underbrace{e^{inx} e^{-imx}}_{e^{i(n-m)x}} dx}_{= \begin{cases} 0 & n \neq m \\ 2\pi & n = m \end{cases}}$$

NB: opposite sign... !

all these terms are $\emptyset$, except for $n = m$

yes! This is the rule: $= c_m$

$$\Rightarrow \boxed{c_n = \frac{1}{2\pi}\int_{-\pi}^{+\pi} f(x)\, e^{-inx}\, dx}$$

easy to see that for real $f(x)$: $c_{-n} = c_n^*$

Please note - sign!

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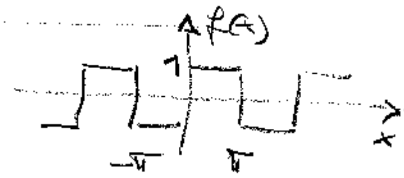
exercise: Find c_n for $f(x) = \begin{cases} 0 & -\pi < x < 0 \\ 1 & 0 < x < \pi \end{cases}$



Solution: ...

$$f(x) = \frac{1}{2} + \frac{1}{i\pi}\left(\frac{e^{ix}}{1} + \frac{e^{3ix}}{3} + \frac{e^{5ix}}{5} + \dots\right) +$$

$$+ \frac{1}{i\pi}\left(\frac{e^{-ix}}{-1} + \frac{e^{-3ix}}{-3} + \frac{e^{-5ix}}{-5} + \dots\right) =$$

$$= \dots = \frac{1}{2} + \frac{2}{\pi}\left(\frac{\sin x}{1} + \frac{\sin 3x}{3} + \frac{\sin 5x}{5} + \dots\right)$$

(same result as before, expressed in a different way)

Example: solution

$$f(x) = \begin{cases} 0 & -\pi < x < 0 \\ 1 & 0 < x < \pi \end{cases}$$

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\, e^{-inx}\, dx = \frac{1}{2\pi}\cancel{\int_{-\pi}^{0} 0 \cdot e^{-inx}\, dx} + \frac{1}{2\pi}\int_{0}^{\pi} 1 \cdot e^{-inx}\, dx =$$

$$= \frac{1}{2\pi}\left[\frac{e^{-inx}}{-in}\right]_0^{\pi} = \frac{1}{-2\pi i n}\cdot\left(e^{-in\pi} - 1\right) = \begin{cases} \frac{1}{\pi i n} & n \text{ odd} \\ 0 & n \text{ even} \end{cases}$$

n odd : $e^{-in\pi} = -1$

n even : $e^{-in\pi} = +1$

$$c_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\, dx = \frac{1}{2\pi}\int_0^{\pi} dx = \frac{1}{2}$$

$$\Rightarrow f(x) = \sum_{n=-\infty}^{+\infty} c_n e^{inx} = \frac{1}{2} + \frac{1}{i\pi}\left(\frac{e^{ix}}{1} + \frac{e^{3ix}}{3} + \frac{e^{5ix}}{5} + \dots\right) + \frac{1}{i\pi}\left(\frac{e^{-ix}}{-1} + \frac{e^{-3ix}}{-3} + \frac{e^{-5ix}}{-5} + \dots\right)$$

$$= \frac{1}{2} + \frac{2}{\pi}\left(\underbrace{\frac{e^{ix} - e^{-ix}}{1 \cdot 2i}}_{\frac{\operatorname{sen} x}{1}} + \underbrace{\frac{e^{i3x} - e^{-i3x}}{3 \cdot 2i}}_{\frac{\operatorname{sen} 3x}{3}} + \dots\right)$$

OK, not so difficult, after all.

4. Other intervals

Please note:

(a) if we are only interested in the finite interval $[-\pi, \pi]$ the function $f(x)$ does not really need to be "intrinsically" periodic: one can always define $f(x)$ outside $[-\pi, \pi]$ so that it is forced to be periodic.

(b) it is easy to extend Fourier series to different intervals

$$[-\pi,\pi] \quad \text{length } 2\pi \qquad \underbrace{\cos nx,\ \sin nx,\ e^{inx}}_{\text{period } 2\pi}$$

$$\left.\begin{array}{lll} \longrightarrow [-\ell, \ell] & \text{"} & 2\ell \\ \longrightarrow [0, 2\ell] & \text{"} & 2\ell \end{array}\right\} \rightarrow \underbrace{\cos n\frac{\pi}{\ell}x,\ \sin n\frac{\pi}{\ell}x,\ e^{in\frac{\pi}{\ell}x}}_{\text{period } 2\ell}$$

"change of variable": $x \rightarrow \frac{\pi}{\ell}x$; for $x = \pm\ell$, $\frac{\pi}{\ell}x = \pm\pi$

$\Rightarrow$ the Fourier series becomes: $\left(\frac{1}{2\pi}\int_{-\pi}^{+\pi} \longrightarrow \frac{1}{2\ell}\int_{-\ell}^{+\ell}\right)$

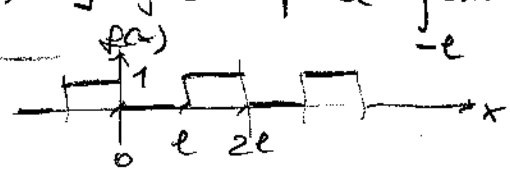
$$f(x) = \frac{1}{2}a_0 + \sum_{1}^{\infty}{}_n\, a_n \cos n\frac{\pi}{\ell}x + \sum_{1}^{\infty}{}_n\, b_n \sin n\frac{\pi}{\ell}x \qquad a_n = \frac{1}{\ell}\int_{-\ell}^{\ell} f(x)\cos n\frac{\pi}{\ell}x\, dx$$

$$b_n = \frac{1}{\ell}\int_{-\ell}^{\ell} f(x)\sin n\frac{\pi}{\ell}x\, dx$$

$$f(x) = \sum_{-\infty}^{+\infty}{}_n\, c_n e^{-in\frac{\pi}{\ell}x} \qquad c_n = \frac{1}{\ell}\int_{-\ell}^{\ell} f(x)\, e^{-in\frac{\pi}{\ell}x}\, dx$$

if the interesting interval is $[0, 2\ell]$ just replace $\int_{-\ell}^{\ell} dx \longrightarrow \int_{0}^{2\ell} dx$

Exercise: $f(x) = \begin{cases} 0 & 0 < x < \ell \\ 1 & \ell < x < 2\ell \end{cases}$



....

Solution: $f(x) = \frac{1}{2} - \frac{2}{\pi}\left(\frac{\sin\frac{\pi}{\ell}x}{1} + \frac{\sin 3\frac{\pi}{\ell}x}{3} + \cdots\right)$

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5. Odd and even functions

Easy to check:

even functions $\Longrightarrow$ $\begin{cases} a_n = \frac{2}{\ell}\int_0^{\ell} f(x) \cos n\frac{\pi}{\ell}x \, dx \\ b_n = 0 \quad \forall n \end{cases}$

$f(-x) = f(x)$

even

"Cosine Fourier Series"

odd functions $\Longrightarrow$ $\begin{cases} a_n = 0 \\ b_n = \frac{2}{\ell}\int_0^{\ell} f(x) \sin n\frac{\pi}{\ell}x \, dx \end{cases}$

$f(-x) = -f(x)$

$\Longrightarrow$ Several different (but equivalent) ways of representing a given function on an interval $[a,b]$ by a Fourier series (cos, sin, exp. ..)

$\Longrightarrow$ choice based on $\begin{cases} \text{period} \\ \text{even/odd} \ldots \end{cases}$

$\leadsto$ in the end, the result is the same series, but there may be shortcuts simplifying the calculations ...!

6. Parseval's theorem ("completeness")

if $f(x)$ complex, then $|f(x)|^2 = f f^*$.

average of $[f(x)]^2$ $\equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} [f(x)]^2 dx = \left(\frac{1}{2}a_0\right)^2 + \sum_1^{\infty} a_n^2 + \sum_1^{\infty} b_n^2$

--- --- $= \sum_{-\infty}^{+\infty} |c_n|^2$

Similar expressions for intervals different from $[-\pi, \pi]$

Note: similarity with vectors, their components and their moduli.

Fourier Transforms

Periodic functions can be expanded in series of sines, cosines, and complex exponentials

(physically: the terms of the expansion can be thought of as representing a set of "harmonics", as in string vibration, sound, AC voltages etc.)

Questions: (1) not periodic functions can be represented by something similar to a Fourier series?

(2) can we extend or modify Fourier series to cover the cases where we have a continuous spectrum, for instance (wavelengths in light, frequencies in sound...)

Answer: the extension is obtained by replacing the Fourier series (a sum) with a Fourier integral to represent $\left\{\begin{array}{l}\text{non periodic functions} \mid \text{sound, pulse of light, voltage pulse...} \\ \text{a continuous set of frequencies..}\end{array}\right.$

$$f(x) = \sum_{-\infty}^{+\infty} c_n e^{in\frac{\pi}{\ell}x}, \quad c_n = \frac{1}{2\ell}\int_{-\ell}^{+\ell} f(x)\, e^{-in\frac{\pi}{\ell}x}\, dx$$

$\hookrightarrow$ (period 2ℓ)

def. "Fourier integral transform"

$$f(x) = \int_{-\infty}^{+\infty} g(\alpha)\, e^{i\alpha x}\, d\alpha, \quad g(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)\, e^{-i\alpha x}\, dx$$

or, equivalently, with a more symmetric definition:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} g(\alpha)\, e^{i\alpha x}\, d\alpha, \quad g(\alpha) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)\, e^{-i\alpha x}\, dx$$

$g(\alpha)$: "Fourier transform" of $f(x)$ (in place of c_n "coefficients")

$f(x)$: "inverse Fourier transform" of $g(\alpha)$

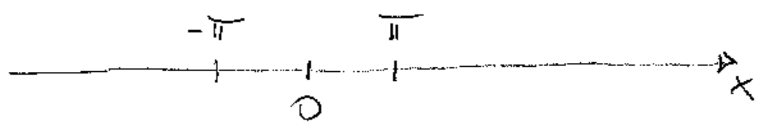
<u>Fourier integral theorem</u> :

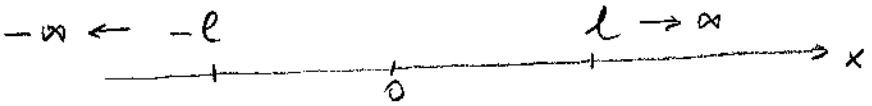
If $f(x)$ satisfies the Dirichlet conditions (see before...) on every finite interval, and if $\int_{-\infty}^{+\infty} |f(x)|\,dx$ is finite, then the transform exists.

(if there are discontinuities / "jumps", the integral gives the midpoint of the jump)

<u>NB</u> We can understand the transition series $\longrightarrow$ integral transform as a limiting process: $[-\ell, \ell] \longrightarrow [-\infty, \infty]$

heuristic proof !!





$$f(x) = \sum_{-\infty}^{+\infty} c_n \, e^{in\frac{\pi}{\ell}x} \qquad \alpha_n = \frac{n\pi}{\ell}$$

$$\alpha_{n+1} - \alpha_n = \frac{\pi}{\ell} = \Delta\alpha \longrightarrow 0$$

$$c_n = \frac{1}{2\ell}\int_{-\ell}^{+\ell} f(x)\, e^{i\alpha_n x}\, dx = \frac{\Delta\alpha}{2\pi}\int_{-\ell}^{\ell} f(u)\, e^{-i\alpha_n u}\, du$$

$$\frac{1}{2\ell} = \frac{1}{2}\,\frac{\pi}{\pi}\,\frac{1}{\ell} = \frac{\Delta\alpha}{2\pi}$$

$$= \sum_{-\infty}^{+\infty}{}_n \frac{\Delta\alpha}{2\pi}\int_{-\ell}^{+\ell} f(u)\, e^{-i\alpha_n u}\, du \cdot e^{i\alpha_n x} =$$

$$= \frac{1}{2\pi}\sum_{-\infty}^{+\infty}{}_n \Delta\alpha \cdot \underbrace{\int_{-\ell}^{+\ell} f(u)\, e^{i\alpha_n(x-u)}\, du}_{\longrightarrow F(\alpha_n)}$$

$$f(x) = \frac{1}{2\pi} \sum_{-\infty}^{+\infty}{}_n \Delta\alpha \cdot \underbrace{\int_{-\ell}^{+\ell} f(u)\, e^{i\alpha_n (x-u)}\, du}_{F(\alpha_n)}$$

now, if we let ℓ go to infinity:

$\ell \to \infty$

$$\sum_{-\infty}^{+\infty}{}_n \underset{\substack{\downarrow \\ 0}}{\Delta\alpha} \cdot \underset{\substack{\downarrow \\ \alpha}}{F(\alpha_n)} \xrightarrow[\ell\to\infty]{} \int_{-\infty}^{+\infty} d\alpha\, F(\alpha)$$

becomes a continuous variable

the sum becomes formally an integral

$$F(\alpha) = \int_{-\infty}^{+\infty} f(u)\, e^{i\alpha(x-u)}\, du$$

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\alpha\, F(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\alpha\, e^{i\alpha x} \underbrace{\int_{-\infty}^{+\infty} du\, f(u)\, e^{-i\alpha u}}$$

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\, f(x)\, e^{-i\alpha x} = g(\alpha)$$

$$\Rightarrow \boxed{\begin{aligned} f(x) &= \int_{-\infty}^{+\infty} g(\alpha)\, e^{i\alpha x}\, d\alpha \\ g(\alpha) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)\, e^{-i\alpha x}\, dx \end{aligned}}$$

NB: one can also split

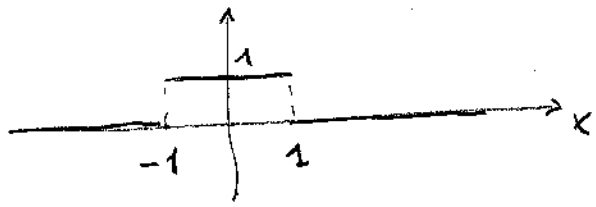
$$\frac{1}{2\pi} = \frac{1}{\sqrt{2\pi}} \cdot \frac{1}{\sqrt{2\pi}}$$

and obtain the "symmetrical" definition

Good. To better appreciate the meaning of the Fourier transform, let us consider two examples.

Example 1

$$f(x) = \begin{cases} 1 & -1 < x < 1 \\ 0 & |x| > 1 \end{cases}$$



(may represent a voltage pulse in circuit theory, or an impulsive force in mechanics, or a pulse of light, etc.)

what is the F.t. $g(\alpha)$?

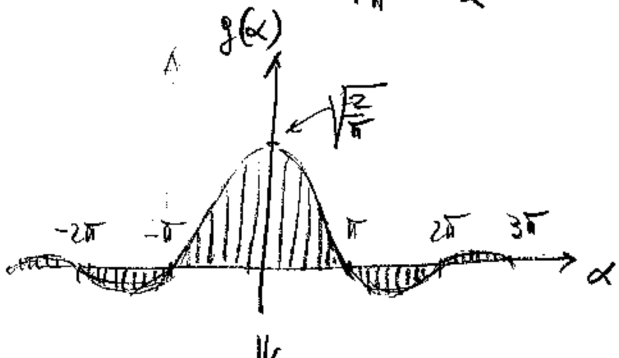
(Physical meaning : "weight" of oscillatory components with continuously varying "frequency" α)

$$g(\alpha) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-i\alpha x}\, dx =$$ ← use the "symmetrical" definition

$$= \frac{1}{\sqrt{2\pi}} \int_{-1}^{+1} e^{-i\alpha x}\, dx =$$

$$= \frac{1}{\sqrt{2\pi}} \left[\frac{e^{-i\alpha x}}{-i\alpha} \right]_{-1}^{+1} = \frac{1}{\sqrt{2\pi}\,\alpha} \; \frac{e^{-i\alpha} - e^{i\alpha}}{-i} = \frac{\sqrt{2}}{\sqrt{\pi}\,\alpha} \; \frac{e^{i\alpha} - e^{-i\alpha}}{2i}$$

$$= \sqrt{\frac{2}{\pi}} \, \frac{\operatorname{sen} \alpha}{\alpha} \qquad \left(\to \frac{1}{\pi} \text{ for } \alpha \to 0 \right)$$



remember :

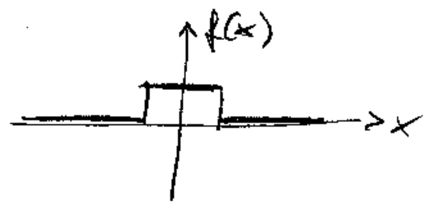
continuous "index" α is now substituting n

"coefficient" $g(\alpha)$ " " c_n

intuitive meaning, explain

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(\alpha) \cdot e^{i\alpha x}\, d\alpha$$

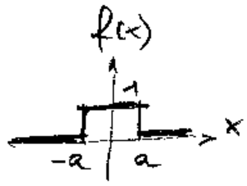
$\Longrightarrow$

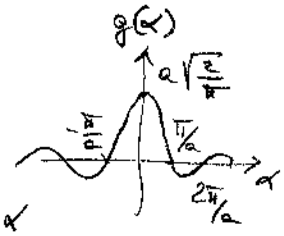


⇒ Table of Fourier transform pairs

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(\alpha)\, e^{i\alpha x}\, d\alpha \qquad g(\alpha) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-i\alpha x}\, dx$$

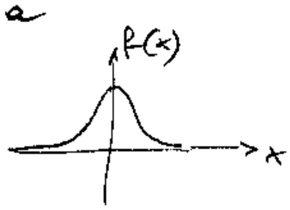
$$f(x) = \begin{cases} 1 & |x| < 1 \\ 0 & |x| > 1 \end{cases} \qquad g(\alpha) = \sqrt{\frac{2}{\pi}}\, \frac{\sin \alpha}{\alpha}$$

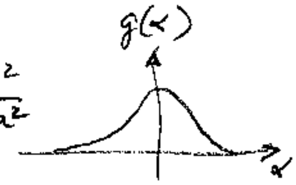




$$f(x) = \begin{cases} 1 & |x| < a \\ 0 & |x| > a \end{cases} \qquad g(\alpha) = \sqrt{\frac{2}{\pi}}\, \frac{\sin a\alpha}{\alpha}$$

$$f(x) = e^{-a^2 x^2} \qquad g(\alpha) = \frac{1}{a\sqrt{2}}\, e^{-\frac{\alpha^2}{4a^2}}$$





(from: A. Jeffrey, Handbook of Mathematical Formulas and Integrals, Academic Press, p.304 (Table 20.1))

Waves, wave packets and one-dimensional wave equation for particles (Schrödinger)

(1) Remember: for e.m. waves, we had found (1-dim.)

$$\frac{\partial^2 \phi(x,t)}{\partial t^2} = \frac{1}{c^2}\frac{\partial^2 \phi(x,t)}{\partial x^2}$$

(ϕ representing e transverse component of the e.m. field)

solution:

$$\phi(x,t) = e^{i(k(x-ct))} = e^{i(kx-\omega_k t)}$$

$$\begin{cases} \omega_k = ck \\ c = \frac{\omega_k}{k} \\ k = \frac{2\pi}{\lambda} \end{cases}$$

one can use, for the classical case,

$$\mathrm{Re}\,\phi(x,t) = \cos(kx-\omega t)$$

Also this is a solution.

NB: for light (e.m. waves) in a vacuum $\frac{\omega_k}{k} = c$ for all frequencies (wavelengths)

(2) A linear superposition of solutions is again a solution, for instance:

$$\phi(x,t) = c_1 e^{ik_1(x-ct)} + c_2 e^{ik_2(x-ct)} + \ldots = \sum_n c_n e^{ik_n(x-ct)}$$

this can be generalized (sum → integral)

(3) $$\phi(x,t) = \int_{-\infty}^{+\infty} dk\; a(k)\, e^{ik(x-ct)}$$

(skip this, take it up later)

"Fourier coefficient" (transform) to be determined by the initial condition at $t=0$

"known" initial pulse at $t=0$ → $$\phi(x,0) = \int_{-\infty}^{+\infty} dk\; a(k)\, e^{ikx}$$

can be computed if $\phi(x,0)$ is known

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

Fourier transform at $t=0$

$a(k)$ "weight" of the monochromatic wave with given $k = \frac{2\pi}{\lambda}$

NB: here we have two pairs of variables: (x and k), (t and ω); we apply Fourier analysis to x and k, and consider then $\omega = \omega(k)$

Let us visualize these "wave packets"

k_0 ; $k_1 = k_0 - \Delta k$, $k_2 = k_0 + \Delta k$ $\Longrightarrow$ $\begin{cases} \omega_0 = c k_0 \\ \omega_1 = c k_1 = c k_0 - \underbrace{c\Delta k}_{\Delta\omega} = \omega_0 + \Delta\omega \\ \omega_2 = c k_2 = c k_0 + \underbrace{c\Delta k}_{+\Delta\omega} = \omega_0 - \Delta\omega \end{cases}$

Start with a simple superposition of just two plane waves at fixed t

$$\frac{\omega_0}{k_0} = c = \frac{\Delta\omega}{\Delta k}$$

$\boxed{\text{at } t=0}$

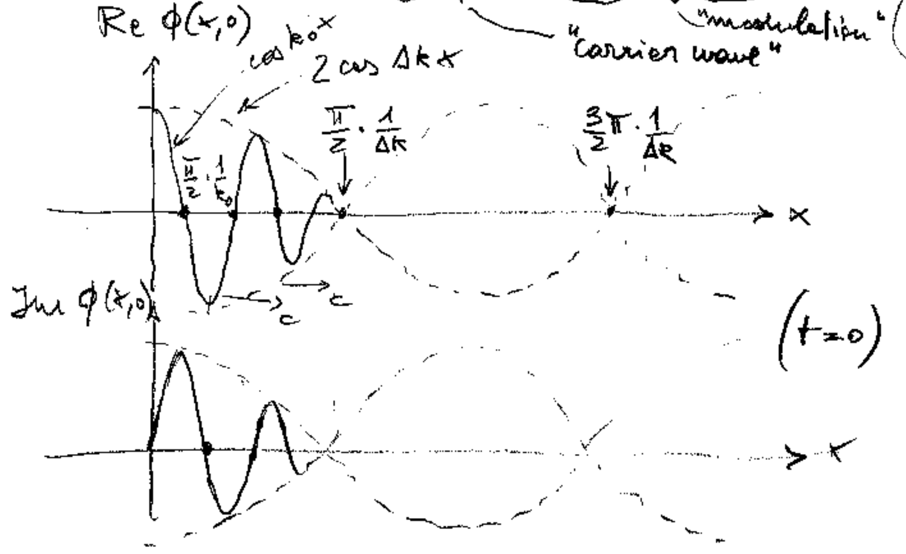
$$\phi(x,0) = e^{ik_1 x} + e^{ik_2 x} =$$

$$= e^{ik_0 x} e^{-i\Delta k x} + e^{ik_0 x} e^{+i\Delta k x} =$$

$$= e^{ik_0 x}\underbrace{\left(e^{i\Delta k x} + e^{-i\Delta k x}\right)} =$$

This is only the space part

$$= \underbrace{e^{ik_0 x}}_{\text{"carrier wave"}} \underbrace{2\cos \Delta k x}_{\text{"modulation"}} = \cos k_0 x \cdot 2\cos\Delta k x + i \sin k_0 x \cdot 2\cos \Delta k x$$



$e^{ik_0 x}$: "carrier"

$\cos \Delta k x$: "amplitude modulation"

let us now introduce also the time dependence:

$\boxed{\text{at } t>0}$:

$$\phi(x,t) = e^{ik_1 x} e^{-i\omega_1 t} + e^{ik_2 x} e^{-i\omega_2 t}$$

$$= \underline{e^{ik_0 x}} e^{-i\Delta k x} \underline{e^{-i\omega_0 t}} e^{+i\Delta\omega t} + \underline{e^{ik_0 x}} e^{+i\Delta k x} \underline{e^{-i\omega_0 t}} e^{-i\Delta\omega t}$$

$$= \underbrace{e^{i(k_0 x - \omega_0 t)}}_{\substack{\text{"carrier wave":} \\ \text{phase velocity } c = \frac{\omega_0}{k_0}}} \cdot \underbrace{e^{i(\Delta k x - \Delta\omega t)} + e^{-i(\Delta k x - \Delta\omega t)}}_{\substack{2\cos(\Delta k x - \Delta\omega t) \\ \text{"amplitude modulation"}}}$$

"group velocity $\frac{\Delta\omega}{\Delta k} = c = \frac{\omega_0}{k_0}$

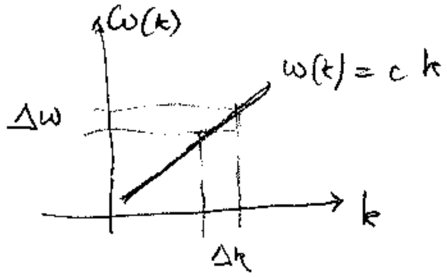
in this case!

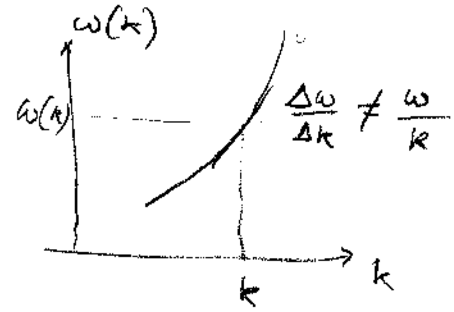
(1) $\Longrightarrow$ in this case $\left(\frac{\omega}{k} = \frac{\Delta\omega}{\Delta k} = c \right.$, e.m. waves in vacuum$\left.\right)$

phase velocity = group velocity (in general this is not true)

carrier wave , modulation move at the same speed!

(2) what happens if $\frac{\omega(k)}{k} \neq \frac{\Delta\omega}{\Delta k}$?





linear relation $\omega(k) = c\,k$

$\Longrightarrow \Delta\omega = c\,\Delta k$

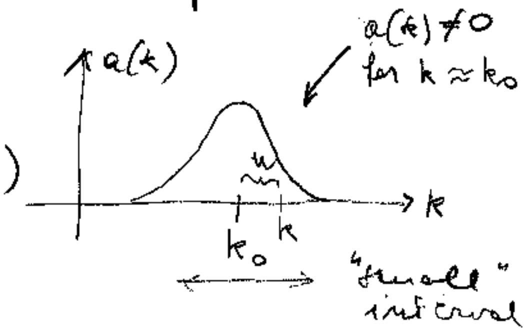
(3) $v_{group} = \frac{\Delta\omega}{\Delta k} \neq \frac{\omega(k)}{k} = v_{phase}$.

"group velocity" $\neq$ phase velocity

in general, if $\omega = \omega(k)$ phase velocity and group velocity are different

(see demo) applets

Phase velocity and group velocity for wave packets with continuous spectrum:



(1) Consider

$$\phi(x,t) = \int_{-\infty}^{+\infty} dk\; a(k-k_0)\, e^{i(kx-\omega_k t)}$$

This is similar to the sum of two plane waves, but generalized to an integral with coefficients varying continuously

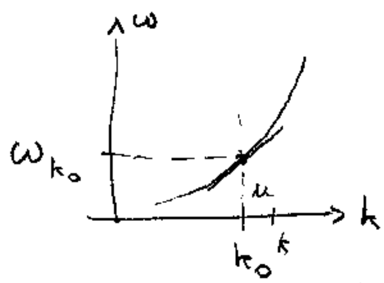
(2) let us show that this wave function $\phi(x,t)$ behaves similarly to the previous case: it can be split in the product of two parts corresponding to:

- a "carrier wave" $e^{i(k_0x-\omega_0 t)}$ $\longleftrightarrow$ propagating with $v_{phase} = \frac{\omega_0}{k_0}$
- a "modulation", propagating at speed $v_{group} = \left.\frac{\partial\omega}{\partial k}\right|_{k_0}$

(3)

$$k \equiv k_0 + \overbrace{(k-k_0)}^{u}$$

$$\omega_k \equiv \omega_{k_0} + \underbrace{(k-k_0)}_{u}\left.\frac{\partial\omega_k}{\partial k}\right|_{k_0} + \dots$$



after introducing the variable $u = k-k_0$ ($\Rightarrow du = dk$) and a Taylor expansion of ω as a function of k near k_0, the wave function becomes:

$$\phi(x,t) = \int_{-\infty}^{+\infty} du\; a(u)\, e^{i(k_0x-\omega_{k_0}t)}\, e^{i\left(ux - u\underbrace{\left(\frac{\partial\omega_k}{\partial k}\right)_{k_0}}_{v_{group}}t\right)} =$$

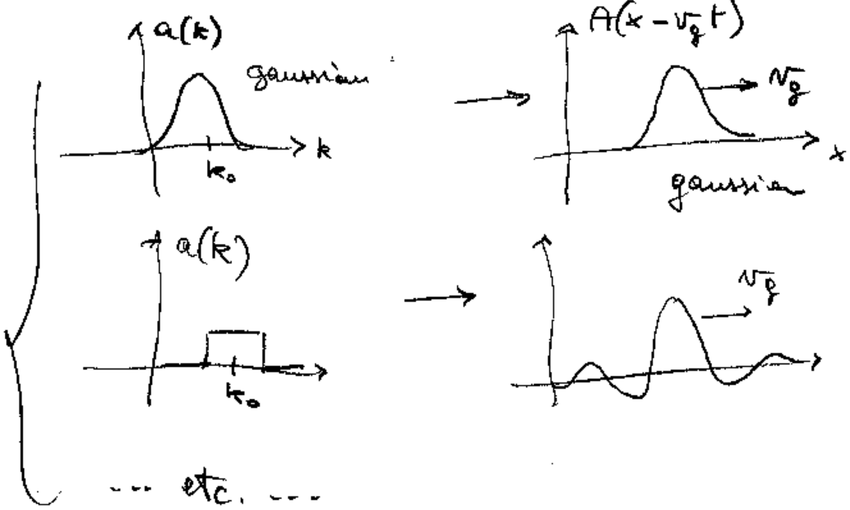
$$= e^{i(k_0x-\omega_{k_0}t)}\int_{-\infty}^{+\infty} du\; a(u)\, e^{i\left[u(x-v_{group}t)\right]}$$

$$\phi(x,t) = \underbrace{e^{i(k_0 x - \omega_{k_0} t)}}_{\text{"carrying wave"}} \quad \underbrace{A(x - v_{group}\, t)}_{\text{"amplitude modulation"}}$$

↑ Fourier transform of $a(k)$ (or $a(u)$)

the exact "shape" of A depends on the "shape" of $a(k)$, see tables of Fourier transforms.

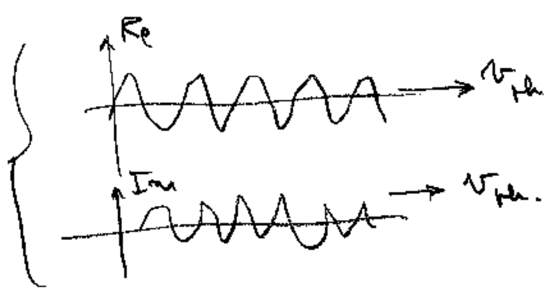
for instance:



How does $\phi(x,t)$ change with time?

① the "carrying wave" moves with "phase velocity"

$$v_{phase} = \frac{\omega_{k_0}}{k_0}$$



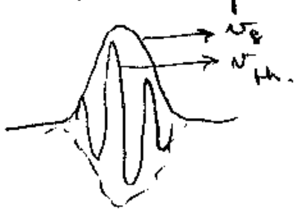
("velocity of a surface with constant phase"

$k_0 x - \omega_{k_0} t = \text{const.}$

$x = \text{const.} + \frac{\omega_{k_0}}{k_0} t$

$v_{phase} = \frac{dx}{dt} = \frac{\omega_{k_0}}{k_0}$)

② the "amplitude modulation" moves with "group velocity"



$$v_{group} = \left(\frac{\partial \omega}{\partial k}\right)_{k_0}$$

NB $v_{group} = v_{phase}$ only if $\omega(k)/k = \text{const.}$