INTRODUCTION TO QUANTUM MECHANICS

PART-II MAKING PREDICTIONS in QUANTUM MECHANICS and the HEISENBERG's PRINCIPLE

CHAPTER-4

WAVEPACKETS
DESCRIPTION OF A FREE-PARTICLE's MOTION

4.3 DESCRIPTION of a FREE PARTICLE MOTION

4.3.A Trial-1: A wavefunction with a definite momentum

4.3.B Trial-2: A wavepacket as a wavefunction

References:

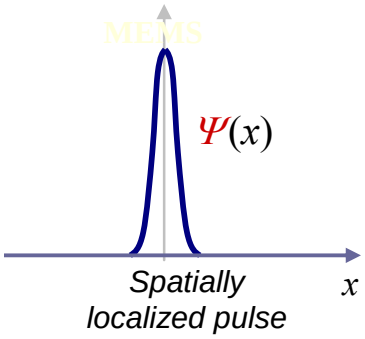
R. Eisberg and R. Resnick, "Quantum Physics," 2nd Edition, Wiley, 1985 **Chapter 3**.

D. Griffiths, "Introduction to Quantum Mechanics"; 2nd Edition, Pearson Prentice Hall. **Chapter 2**.

CHAPTER-4
WAVEPACKET
MOTION DESCRIPTION of a FREE-PARTICLE

In an effort to reach a better understanding of the wave-particle duality, the motion of a free-particle will be described by a **wave packet** $\Psi = \Psi(x,t)$ composed of traveling harmonic waves [the latter have the form $Sin(kx-\omega t)$, $Cos(kx-\omega t)$].

$$\Psi(x,t) = \sum_k A(k) Sin\,[kx - \omega(k)t]$$



A wavepacket is a function whose values, at a given time, are different from zero only in a limited spatial region of extension Δx. If a wavepacket of width Δx were to represent a particle, Δx is then interpreted as the spread spatial location where the particle may be located (i.e. there is an uncertainty about its "exact" location.)

4.1 SPECTRAL DECOMPOSITION OF A FUNCTION (relative to a basis-set of functions)

The approach of describing a wave-profile $\Psi(x)$ as the sum of harmonic waves is formally known spectral Fourier analysis.

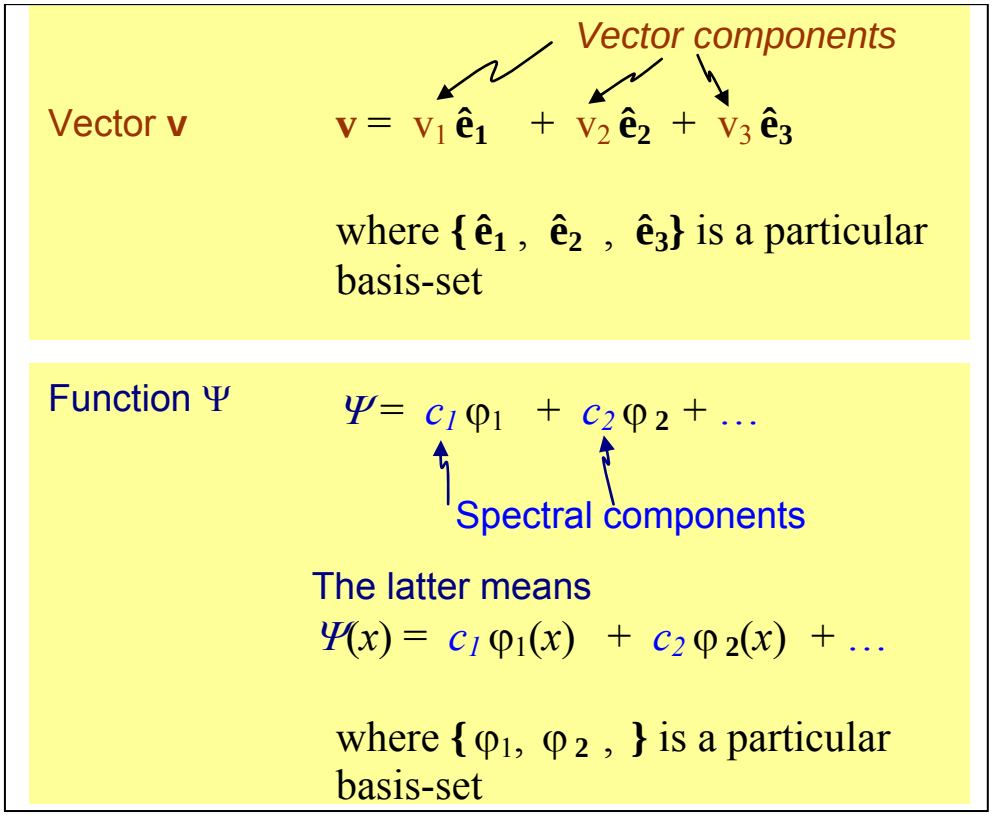
The Fourier analysis (based on harmonic waves) is, however, a particular case of a broader mathematical approach that describes a given function Ψ as a linear combination of a well defined set of

basis-functions { φ_1 , φ_2 , φ_3 , ... }.

In the particular case that the basis-set is chosen to be composed of harmonic functions then the Fourier analysis results. But, in general, different types of basis sets do exist. In what follows we will provide a view of this more general description since it will allow us to provide different optional descriptions of quantum mechanics phenomena.

4.1.A Analogy between the components of a vector V and spectral components of a function Ψ

Let's consider the analogy between the components of a three dimensional vector, and the spectral decomposition of an arbitrary function Ψ.



(1)

Vector components

In the expression (1) above,

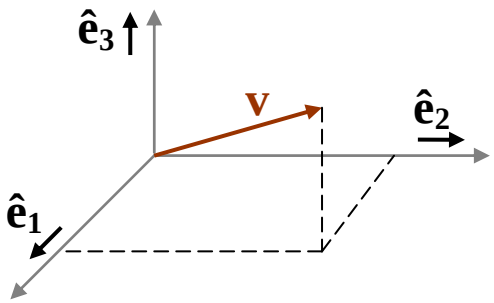
$$\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\} \qquad (2)$$

is a set of unit vectors perpendicular to each other; that is,

$$\hat{\mathbf{e}}_i \bullet \hat{\mathbf{e}}_j = \delta_{ij} \qquad (3)$$

where $\delta_{ij} \equiv 0$ if $j \neq i$

$\equiv 1$ if $j = i$



How to find the components of a vector **v** ?

- If, for example a vector **v** were expressed as

  $\mathbf{v} = 3\,\hat{\mathbf{e}}_1 + 7\,\hat{\mathbf{e}}_2 - 2\,\hat{\mathbf{e}}_3$,

  then, its component would be given by

  $\hat{\mathbf{e}}_1 \bullet \mathbf{v} = 3$; $\hat{\mathbf{e}}_2 \bullet \mathbf{v} = 7$; and $\hat{\mathbf{e}}_3 \bullet \mathbf{v} = -2$

- In a more general case,

  if $\mathbf{v} = v_1\,\hat{\mathbf{e}}_1 + v_2\,\hat{\mathbf{e}}_2 + v_3\,\hat{\mathbf{e}}_3$

  its components v_j are obtained by

  $v_j = \hat{\mathbf{e}}_j \bullet \mathbf{v} = v_j$; for j=1, 2,3

  Thus, $\mathbf{v} = \sum_{j=1}^{3} (\hat{\mathbf{e}}_j \bullet \mathbf{v})\,\hat{\mathbf{e}}_j$ (4)

Notice the involvement of the scalar product to obtain the components of a vector. For the effect of describing the spectral components of a function we similarly introduce in the following section a type of scalar product between functions.

4.1.B The scalar product between two *periodic* functions

Set of base functions. In the expression (1) above, we assume that

$\{ \varphi_1 , \varphi_2 , \varphi_3 , \ldots \}$ (5)

is a infinite basis-set of given functions perpendicular to each other.

That is,

$\varphi_i \bullet \varphi_j = \delta_{ij}$

But what would $\varphi_i \bullet \varphi_j$ mean?

To answer this question, let's consider the particular case where all the functions under consideration are periodic and real; let λ be the periodicity of the functions;

$$\Psi(x+\lambda) = \Psi(x) \qquad (6)$$

Definition. A scalar product between two periodic (but otherwise arbitrary) real functions Ψ and Φ is defined as follows,

$$\Psi \bullet \Phi \equiv \int_0^{\lambda} \psi(x)\, \Phi(x) dx$$

(Throughout these lecture notes, the symbol " $\equiv$ " means *"definition"*).

Rather than using $\Psi \bullet \Phi$, a more common notation is $(\psi\ , \Phi)$

$$(\psi, \Phi) \equiv \int_0^{\lambda} \psi(x)\, \Phi(x) dx \quad \textit{definition of "scalar product" (for the case of real functions)} \qquad (7)$$

In Section 4.1.F below, we extend this definition to include functions whose values lie in the complex variable domain.

Orthogonally property. As mentioned above, the set of base functions indicated in (5) are typically chosen in such a way as to have the following property,

$$\left(\varphi_i\ , \varphi_j \right) \equiv \int_0^{\lambda} \varphi_i(x) \varphi_j(x) dx = \delta_{ij} \qquad (8)$$

Exercise: Given the functions,

$\varphi(x) = \text{Cos}(x)$ and $\Psi(x) = \text{Sin}(x)$,

defined over the range $(0, 2\pi)$,

evaluate the scalar product $(\varphi\ ,\ \Psi)$.

Answer: $\int_0^{2\pi} Cos(x)\, Sin\,(x) dx = 0$

Bracket notation. Dirac introduced a bracket notation, where the scalar product is denoted by

$\langle \psi | \Phi \rangle$ instead of (ψ, Φ)

Still the parenthesis notation is much more clear and straightforward. The bracket notation however offers (as we will see in the next chapters) great flexibility and simplification to (when properly used) represent both states and operators (as far as the distinction between states and operators is implicitly understood). But occasionally the bracket notation will present difficulties on how to use it. When such cases arise, we will resort back to the parenthesis notation for clarification. Since the bracket notation is so broad spread in quantum mechanics we will frequently use it in this course.

4.1.C How to find the spectral components of a function Ψ?

Given an arbitrary periodic function Ψ we wish to express it as a linear combination of the periodic base functions φ_j,

$$\Psi = c_1 \varphi_1 + c_2 \varphi_2 + \ldots \tag{9}$$

Using the scalar product definition given in (9) we can obtain the corresponding values of the coefficients c_j in the following manner (adopting the bracket notation for the scalar product),

$$c_j = \langle \varphi_j | \psi \rangle = \int_0^{\lambda} \varphi_j(x)\, \psi(x) dx \qquad \textit{for j= 1,2,3, …} \tag{10}$$

Still one question remains: How do the functions φ_j look like?

Answer:

- There exist different types of sets. They are even defined with very much generality in quantum mechanics, as we will see when describing an electron traveling in a lattice of atoms (Chapter 7).
- One particular set is the one composed by *harmonic functions*

BASE SET $\{ \mathrm{Cos}_o,\ \mathrm{Cos}_1,\ \mathrm{Sin}_1,\ \mathrm{Cos}_2,\ \mathrm{Sin}_2,\ \ldots \}$

where

$$\mathrm{Cos}_o(x) \equiv \sqrt{\frac{1}{\lambda}}$$

$$\mathrm{Cos}_n(x) \equiv \sqrt{\frac{2}{\lambda}}\,\mathrm{Cos}\left(\frac{2\pi}{\lambda/n}x\right); \qquad \text{for } n=1, 2, \ldots$$

$$\mathrm{Sin}_n(x) \equiv \sqrt{\frac{2}{\lambda}}\,\mathrm{Sin}\left(\frac{2\pi}{\lambda/n}x\right); \qquad \text{for } n=1, 2, \ldots$$

(11)

which are useful to describe any periodic function Ψ of period equal to λ.

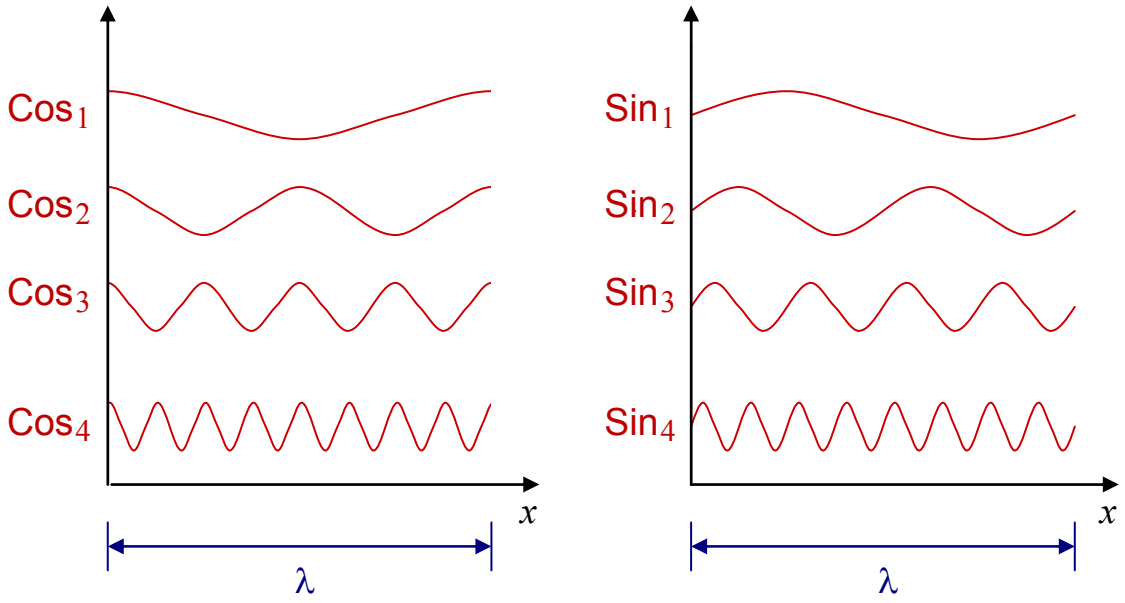


Fig. 4.1 Set of harmonic functions defined in expression (11). They are used as a base to express any periodic function of periodicity equal to λ.

It can be directly verified, using the definition of scalar product given in (10), that the harmonic functions defined in (11) satisfy

$$< \mathrm{Cos}_n \,|\, \mathrm{Sin}_m > = \int_0^{\lambda} Cos_n(x)\, Sin_m(x)dx > \ = 0$$

More generally,

$$
\left.
\begin{aligned}
&\langle \mathrm{Cos}_n \,|\, \mathrm{Sin}_m \rangle = 0 && \text{for arbitrary integers m , n;} \\
&\langle \mathrm{Cos}_n \,|\, \mathrm{Cos}_m \rangle = \delta_{nm} && \text{for arbitrary integers m , n;} \\
&\langle \mathrm{Sin}_n \,|\, \mathrm{Sin}_m \rangle = \delta_{nm} && \text{for arbitrary integers m , n.}
\end{aligned}
\right\} \qquad (12)
$$

4.1.C.a Spectral decomposition of periodic functions
The Series Fourier Theorem

Using the base-set of harmonic functions defined in (11) above, the following theorem results:

A function Ψ of period λ can be expressed as,

$$\Psi(x) = A_o \mathrm{Cos}_o(x) + \sum_{n=1}^{\infty} A_n \mathrm{Cos}_n(x) + \sum_{n=1}^{\infty} B_n \mathrm{Sin}_n(x)$$

or simply

$$\Psi = A_o \mathrm{Cos}_o + \sum_{n=1}^{\infty} A_n \mathrm{Cos}_n + \sum_{n=1}^{\infty} B_n \mathrm{Sin}_n \qquad (13)$$

where the coefficient are given by

$$A_n = \langle \mathrm{Cos}_n \,|\, \Psi \rangle = \int_0^{\lambda} Cos_n(x)\,\psi(x)dx \qquad n = 0,1,2, \ldots$$

$$B_n = \langle \mathrm{Sin}_n \,|\, \Psi \rangle = \int_0^{\lambda} Sin_n(x)\,\psi(x)dx \qquad n = 1,2, \ldots \qquad (14)$$

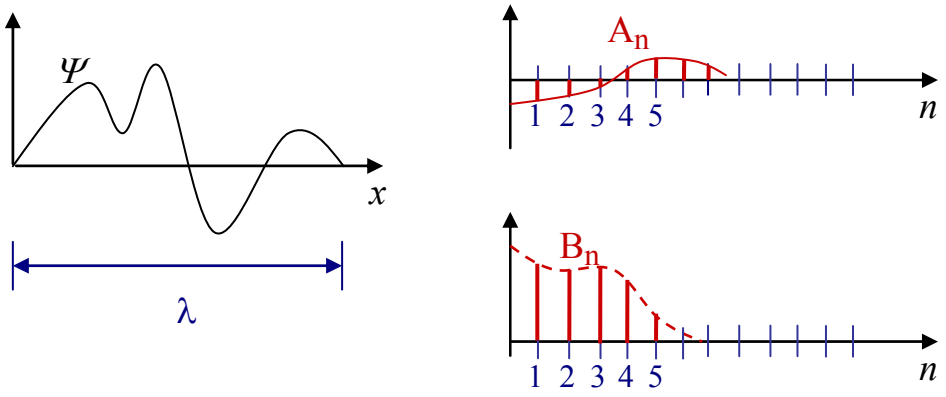


Fig. 4.2 Periodic function Ψ and its corresponding Fourier spectrum fingerprint

Notice

- in expression (13) above the explicit dependence of the functions on the variable x can be omitted. That is, we can work simply and directly with the functions Cos_n instead of working with the numbers $\mathrm{Cos}_n(x)$, whenever convenient.
- In the notation for the scalar product we use $<\mathrm{Cos}_n|\Psi>$ and not $<\mathrm{Cos}_n(x)|\Psi(x)>$. This is to emphasize that the scalar product is between functions and not between numbers.
- Using explicitly the expression for $\mathrm{Cos}_o=\sqrt{\frac{1}{\lambda}}$ and, according to (13), $A_0=<\mathrm{Cos}_o|\Psi> = \int_0^{\lambda} Cos_o(x)\,\psi(x)dx = \int_0^{\lambda}\sqrt{\frac{1}{\lambda}}\,\psi(x)dx$ we realize that the first term in the Fourier series expansion is nothing but the average value (average taken over one period) of the function Ψ. That is,

$$\Psi(x) = \frac{1}{\lambda}\int_0^{\lambda}\psi(x')dx' + \sum_{n=1}^{\infty} A_n\,\mathrm{Cos}_n(x) + \sum_{n=1}^{\infty} B_n\,\mathrm{Sin}_n(x) \qquad (15)$$

4.1.C.b Spectral decomposition of *Non-periodic* Functions. The Fourier Integral

The series Fourier expansion allows the analysis of periodic functions, where λ specifies the periodicity. For the case of non-periodic functions a similar analysis is pursued by taking the limit when $\lambda \to \infty$.

For an arbitrary function Ψ of period λ we have the Fourier series expansion,

$$\Psi(x) = A_o\,\mathrm{Cos}_o(x) + \sum_{n=1}^{\infty} A_n\,\mathrm{Cos}_n(x) + \sum_{n=1}^{\infty} B_n\,\mathrm{Sin}_n(x)$$

Writing the base-functions in a more explicit form (using expression (11)), one obtains,

$$\Psi(x) = \frac{1}{\lambda}\int_0^{\lambda}\psi(x)dx + \sum_{n=1}^{\infty} A_n \underbrace{\sqrt{\frac{2}{\lambda}}\,\mathrm{Cos}\left(\frac{2\pi}{\lambda/n}x\right)}_{\mathrm{Cos}_n(x)} + \sum_{n=1}^{\infty} B_n \underbrace{\sqrt{\frac{2}{\lambda}}\,\mathrm{Sin}\left(\frac{2\pi}{\lambda/n}x\right)}_{\mathrm{Sin}_n(x)}$$

Since Ψ and all the harmonic functions have period λ, we can change the interval of interest $(0, \lambda)$ to $(-\lambda/2, \lambda/2)$ and thus re-write,

$$\Psi(x) = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2}\psi(x')dx' + \sum_{n=1}^{\infty} A_n \underbrace{\left[\sqrt{\frac{2}{\lambda}}\mathrm{Cos}\left(n\frac{2\pi}{\lambda}x\right)\right]}_{\mathrm{Cos}_n(x)} + \sum_{n=1}^{\infty} B_n \underbrace{\left[\sqrt{\frac{2}{\lambda}}\mathrm{Sin}\left(n\frac{2\pi}{\lambda}x\right)\right]}_{\mathrm{Sin}_n(x)}$$

$$\textit{where}\quad A_n = \langle \mathrm{Cos}_n \mid \Psi \rangle = \int_{-\lambda/2}^{\lambda/2}\left[\sqrt{\frac{2}{\lambda}}\mathrm{Cos}\left(n\frac{2\pi}{\lambda}x'\right)\right]\psi(x')dx\,;\quad n=1,2,\ldots$$

$$B_n = \langle \mathrm{Sin}_n \mid \Psi \rangle = \int_{-\lambda/2}^{\lambda/2}\left[\sqrt{\frac{2}{\lambda}}\mathrm{Sin}\left(n\frac{2\pi}{\lambda}x'\right)\right]\psi(x')dx\,;\quad n=1,2,\ldots$$

Let's define

$$k_o \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad k = nk_o \tag{16}$$

In terms of which the previous expression adopts the form,

$$\Psi(x) = \frac{1}{\lambda}\int_{-\lambda/2}^{\lambda/2}\psi(x')dx' + \sum_{n=1}^{\infty} A_n\left[\sqrt{\frac{2}{\lambda}}\mathrm{Cos}(nk_0x)\right] + \sum_{n=1}^{\infty} B_n\left[\sqrt{\frac{2}{\lambda}}\mathrm{Sin}(nk_0x)\right]$$

$$\text{where}\quad A_n = \langle \mathrm{Cos}_n \mid \Psi \rangle = \int_{-\lambda/2}^{\lambda/2}\left[\sqrt{\frac{2}{\lambda}}\mathrm{Cos}(nk_0x')\right]\psi(x')dx\,;\quad n=1,2,\ldots$$

$$B_n = \langle \mathrm{Sin}_n \mid \Psi \rangle = \int_{-\lambda/2}^{\lambda/2}\left[\sqrt{\frac{2}{\lambda}}\mathrm{Sin}(nk_0x')\right]\psi(x')dx\,;\quad n=1,2,\ldots$$

From the (discrete) variable *n* to the (continuum) *k* variable

When $\lambda \to \infty$, the value $k_o \equiv \frac{2\pi}{\lambda} \to 0$ and the summation over n becomes an Integral of the variable $k = nk_o$. In a range Δk there will be an integer number $(\Delta k)/k_o$ of terms that in the summation above will have a similar coefficient A_n.

It is also convenient to use the index k instead of n: A_n becomes A_k

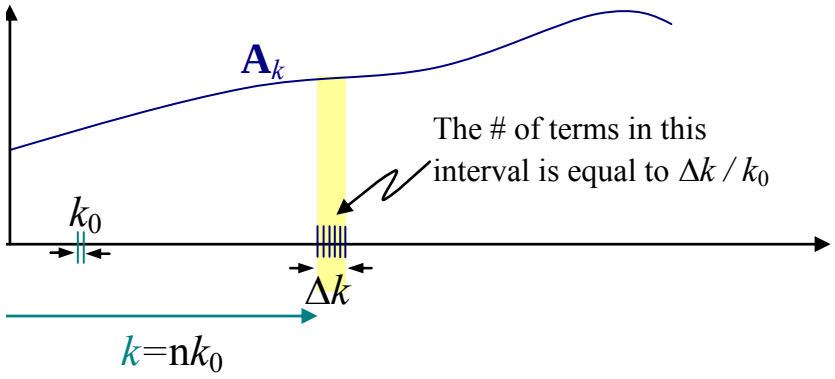


Fig. 4.3 Transition of the Fourier component from discrete variable n to a continuum variable k.

Thus, as $\lambda \to \infty$ the last expression becomes,

$$\Psi(x) \xrightarrow[\lambda \to \infty]{} \int_0^\infty \frac{\Delta k}{k_o} A_k \left[\sqrt{\frac{2}{\lambda}}\,\mathrm{Cos}(kx)\right] + \int_0^\infty \frac{\Delta k}{k_o} B_k \left[\sqrt{\frac{2}{\lambda}}\,\mathrm{Sin}(kx)\right] \quad (17)$$

where

$$A_n \xrightarrow[\lambda \to \infty]{} A_k = \int_{-\lambda/2}^{\lambda/2} \left[\sqrt{\frac{2}{\lambda}}\,\mathrm{Cos}(kx')\right] \psi(x')dx'$$

$$B_n \xrightarrow[\lambda \to \infty]{} B_k = \int_{-\lambda/2}^{\lambda/2} \left[\sqrt{\frac{2}{\lambda}}\,\mathrm{Sin}(kx')\right] \psi(x')dx'$$

Replacing the coefficients A_k and B_k in (17) itself,

$$\Psi(x) \xrightarrow[\lambda \to \infty]{} \int_0^{\infty} \frac{\Delta k}{k_o} \underbrace{\left[\sqrt{\frac{2}{\lambda}} \int_{-\lambda/2}^{\lambda/2} \mathrm{Cos}(kx')\, \psi(x')dx'\right]}_{A_k} \left[\sqrt{\frac{2}{\lambda}}\, \mathrm{Cos}(kx)\right] +$$

$$+ \int_0^{\infty} \frac{\Delta k}{k_o} \underbrace{\left[\sqrt{\frac{2}{\lambda}} \int_{-\lambda/2}^{\lambda/2} \mathrm{Sin}(kx')\, \psi(x')dx'\right]}_{B_k} \left[\sqrt{\frac{2}{\lambda}}\, \mathrm{Sin}(kx)\right]$$

Since $\frac{1}{k_o}\sqrt{\frac{2}{\lambda}}\sqrt{\frac{2}{\lambda}} = \frac{1}{\pi}$, a further simplification is obtained,

$$\Psi(x) \xrightarrow[\lambda \to \infty]{} \int_0^{\infty} \Delta k \left[\frac{1}{\pi} \int_{-\lambda/2}^{\lambda/2} \mathrm{Cos}(kx')\, \psi(x')dx'\right] \mathrm{Cos}(kx) +$$

$$+ \int_0^{\infty} \Delta k \left[\frac{1}{\pi} \int_{-\lambda/2}^{\lambda/2} \mathrm{Sin}(kx')\, \psi(x')dx'\right] \mathrm{Sin}(kx)$$

$$\left.\begin{aligned} \Psi(x) = & \int_0^{\infty} dk \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{Cos}(kx')\, \psi(x')dx'\right] \mathrm{Cos}(kx) + \\ & + \int_0^{\infty} dk \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{Sin}(kx')\, \psi(x')dx'\right] \mathrm{Sin}(kx) \end{aligned}\right\} \qquad (18)$$

Or, equivalently

$$\Psi(x) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} dk \underbrace{\left[\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{Cos}(kx')\, \psi(x')dx'\right]}_{A(k)} \mathrm{Cos}(kx) +$$

$$+ \frac{1}{\sqrt{\pi}} \int_0^{\infty} dk \underbrace{\left[\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{Sin}(kx')\, \psi(x')dx'\right]}_{B(k)} \mathrm{Sin}\,(kx)$$

Thus, using the BASIS-SET

$$\{\ \mathrm{Cos_k}\ ,\ \mathrm{Sin_k}\ ;\quad 0 < \mathrm{k} < \infty\ \} \tag{19}$$

where

$$\mathrm{Cos_k}(x) \equiv \mathrm{Cos(k}x) \quad \textit{and} \quad \mathrm{Sin_k}(x) \equiv \mathrm{Cos(k}x)$$

we have demonstrated that an arbitrary periodic function $\Psi(x)$ can be expressed as a linear combination of such basis-set functions,

$$\Psi(x) = \frac{1}{\sqrt{\pi}} \int_0^\infty \underbrace{A(k)}\ \mathrm{Cos_k}(x)\, dk \ + \ \frac{1}{\sqrt{\pi}} \int_0^\infty \underbrace{B(k)}\ \mathrm{Sin_k}(x)\, dk \tag{20}$$

Fourier coefficients

where the amplitude coefficients of the harmonic functions components are given by,

$$A(k) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \psi(x')\, \mathrm{Cos}(kx')dx', \quad \text{and}$$

$$B(k) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \psi(x')\, \mathrm{Sin}(kx')dx'$$

4.1.D Spectral decomposition in complex variable. The Fourier Transform.

In expression (18) above we have

$$\Psi(x) = \int_0^\infty dk \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{Cos}(kx')\ \psi(x')dx'\right] \mathrm{Cos}(kx) \ +$$

$$+ \int_0^\infty dk \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{Sin}(kx')\ \psi(x')dx'\right] \mathrm{Sin}(kx)$$

which can be expressed as,

$$\Psi(x) = \int_0^\infty dk \, \frac{1}{\pi} \int_{-\infty}^{\infty} \{ \text{Cos}\ (kx') \, \text{Cos}(kx) \} \, \psi(x') dx' \; +$$

$$+ \int_0^\infty dk \, \frac{1}{\pi} \int_{-\infty}^{\infty} \{ \text{Sin}(kx') \, \text{Sin}(kx) \} \, \psi(x') dx'$$

$$\Psi(x) = \int_0^\infty dk \, \frac{1}{\pi} \int_{-\infty}^{\infty} \{ \text{Cos}(k(x'-x) \} \, \psi(x') dx'$$

In the expression above one can identify an even function in the variable k,

$$\Psi(x) = \int_0^\infty dk \, \underbrace{\left[\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Cos}(k(x'-x) \, \psi(x') dx' \right]}_{\text{Even function in the variable } k} \tag{21}$$

accordingly, we have the following equality

$$\int_0^\infty dk \, \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Cos}(k(x'-x) \, \psi(x') dx' \right] = \tag{22}$$

$$= \int_{-\infty}^{0} dk \, \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Cos}(k(x'-x) \, \psi(x') dx' \right]$$

(notice the different range of integration in each integral).

Thus, expression (21) can be re-written as,

$$\Psi(x) = \frac{1}{2} \int_{-\infty}^{\infty} dk \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Cos}(k(x'-x) \, \psi(x') dx' \right] \tag{23}$$

On the other hand, notice the following identity

$$0 = - i \frac{1}{2} \int_{-\infty}^{\infty} dk \, \left[\frac{1}{\pi} \int_{-\infty}^{\infty} \text{Sin}(k(x'-x) \, \psi(x') dx' \right] \tag{24}$$

where i is the complex number satisfying i^2= -1. This follows from the fact that the function within the bracket is an odd function with respect to the variable k.

From (23) and (24) we obtain

$$\Psi(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} \underbrace{[\mathrm{Cos}\,(k(x'-x) - i\ \mathrm{Sin}\,(k(x'-x)]}_{e^{-ik(x'-x)}} \psi(x')dx'$$

$$\psi(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} [e^{-ik(x'-x)}]\psi(x')dx' \qquad (25)$$

Rearranging the terms,

$$\Psi(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\ e^{ikx} \int_{-\infty}^{\infty} [e^{-ikx'}\ \psi(x')dx']$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \underbrace{\{\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} [e^{-ikx'}\ \psi(x')dx']\}}_{F(k)} e^{ikx}\ dk$$

Thus, using the infinite basis-set of complex functions

BASIS-SET $\{ e_k\ ,\quad -\infty < k < \infty \}$ (26)

where $e_k(x) \equiv e^{ikx}$

an arbitrary function Ψ can be expressed as a linear combination of such basis-set functions,

$$\Psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \underbrace{F(k)}_{\text{Fourier coefficients}}\ \underbrace{e^{ikx}}_{\text{Base-functions}}\ dk \qquad (27)$$

where the weight coefficients F(k) of the complex harmonic functions components are given by,

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx'} \psi(x') dx' \qquad (28)$$

which is typically referred to as the Fourier transform of the function Ψ.

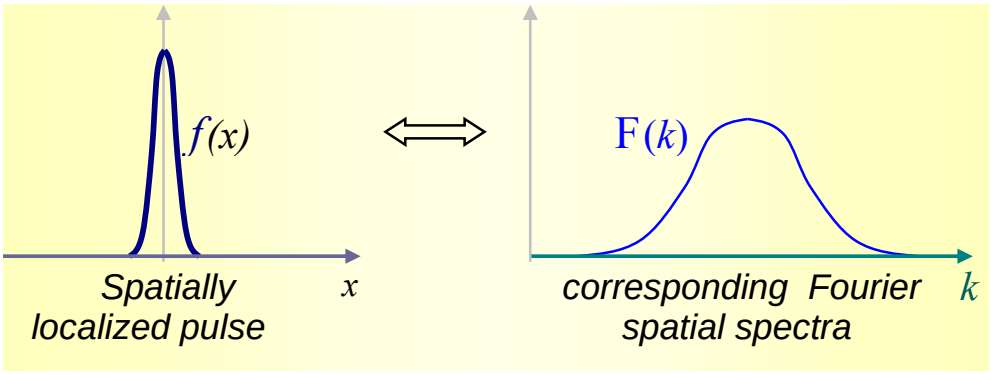
In essence, the Fourier formalism associates to a given function f its Fourier transform F.

$$f \iff F$$

4.1.E Correlation between localized-functions $f = f(x)$ and spread-Fourier (spectral) transforms $F = F(k)$

A fundamental characteristic in the Fourier formalism is that, it turns out,

the more localized is the function f, the broader its spectral Fourier transform F*(k); and vice versa.* (29)



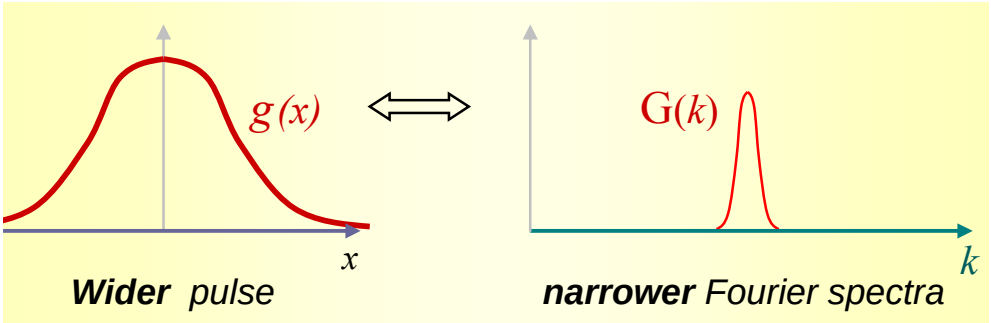


Fig. 4.4 Reciprocity between a function and its spectral Fourier transform

Due to its important application in quantum mechanics, this property will be described in greater detail in the Section 4.2 below. It is worth to emphasize here, however, that the property expressed in (29) has nothing to do with quantum mechanics. It is rather an intrinsic property of the Fourier analysis of waves. However, by identifying (via the de Broglie hypothesis) some variables in the mathematical Fourier description of waves with corresponding physical variables characterizing a particle (*i.e.* position, linear momentum, etc), a better understanding of the quantum mechanical description of the world at the atomic level can be obtained.

4.1.F The Scalar Product in Complex Variable

We will realize through the development of the coming chapters, that the quantum mechanics formalism requires the use of complex variables. Accordingly, let's extend the definition of scalar product to the case where the intervening functions are complex.

Let Φ and ψ be two arbitrary complex functions. The scalar product between Φ and ψ is defined as follows,

$$\langle \Phi | \psi \rangle \equiv \int_{-\infty}^{\infty} \Phi^*(x)\ \psi(x) dx \qquad \textit{definition of scalar product} \tag{30}$$

where the symbol * stands for the complex conjugate. (For example, if $\Phi = a + ib$ then $\Phi^* = a - ib$.)

Notice, $\langle \Phi | \psi \rangle^* = \left[\int_{-\infty}^{\infty} \Phi^*(x)\psi(x)dx \right]^* = \int_{-\infty}^{\infty} [\Phi^*(x)\psi(x)]^* dx = \int_{-\infty}^{\infty} [\Phi(x)\psi^*(x)]dx$;

that is,

$$\langle \Phi | \psi \rangle^* = \langle \psi | \Phi \rangle \tag{31}$$

4.1.G Notation using Bra-kets

The description of some other common notations used in quantum mechanics books is in order.

Particular case: Expansions in Fourier components

- Consider $\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{F(k)e}^{ikx}\, dk$.

  Notice that the corresponding Fourier-transform coefficient $\mathrm{F(k)} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx'}\, \Psi(x')\, dx' = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\mathrm{e}^{ikx'})^{*}\, \Psi(x')\, dx'$ can also be expressed in a more compact form (using the notation for scalar product) as

  $$\mathrm{F(k)} = \frac{1}{\sqrt{2\pi}} \langle \mathrm{e_k} \mid \Psi \rangle \qquad (32)$$

  where $\mathrm{e_k}(x) \equiv \mathrm{e}^{ikx}$

- It is also very common to, alternatively, express the wavefunction $\Psi = \Psi(x)$ in the brackets notation $|\psi\rangle$,

  $$\psi \quad \longleftrightarrow^{\textit{equally represented by}} \quad |\psi\rangle$$

  where all reference to the dependence on the spatial variable x is removed (or implicitly understood.)

  For example, a base function $\frac{1}{\sqrt{2\pi}} \mathrm{e}^{ikx}$ can be represented by a "ket" $|\frac{1}{\sqrt{2\pi}} \mathrm{e_k}\rangle$.

  Further, the "ket" $|\frac{1}{\sqrt{2\pi}} \mathrm{e_k}\rangle$ is sometimes (if not often) simply denoted by $|k\rangle$. (In the latter it is understood that the true meaning is the one given by the former.)

More general case: Expansions in the base $\{\varphi_n;\ n = 1,2,\ \ldots\}$.

- The expression $\Psi(x) = \sum_n A_n\, \varphi_n(x)$

  implies that the function Ψ is a linear combination of the base-functions $\{\varphi_n;\ n = 1,2,\ \ldots\}$. Thus, we can use the notation,

$$\Psi = \sum_n A_n \varphi_n \qquad \text{o r} \qquad |\Psi\rangle = \sum_n A_n |\varphi_n\rangle \tag{33}$$

neither of which allude to the dependence on the spatial variable.

This latter notation is very convenient since there are quantum systems whose wavefunction does not admit a spatial variable dependence (the spin, is a peculiar case.)

For convenience (as we will see later in this course), it would be convenient to use the coefficient A_n on the right side of $|\varphi_n\rangle$;

$$|\Psi\rangle = \sum_n |\varphi_n\rangle A_n \tag{33}'$$

- Another alternative notation or (34) is obtained by expressing A_n in terms of the scalar product.

  In effect, since the basis is orthogonal and normalized basis

  $$\langle \varphi_n | \varphi_m \rangle = \delta_{mn}$$

  then the expansion $|\Psi\rangle = \sum_n |\varphi_n\rangle A_n$ implies

  $$\langle \phi_n | \Psi \rangle = A_n \tag{34}$$

  Accordingly,

  $$|\Psi\rangle = \sum_n |\varphi_n\rangle A_n = \sum_n |\phi_n\rangle \langle \varphi_n | \Psi \rangle \tag{35}$$

4.2 PHASE VELOCITY and GROUP VELOCITY

4.2.A Planes

Let $\vec{\mathbf{r}} = (x,y,z)$ and $\hat{\mathbf{n}}$ be the spatial coordinates and a unit vector, respectively.

Notice,

$$\vec{\mathbf{r}} \cdot \hat{\mathbf{n}} = const$$

locates the points $\vec{\mathbf{r}}$ that constitute a plane perpendicular to $\hat{\mathbf{n}}$.

Different planes are obtained when using different values for the constant value (as seen in the figure below).

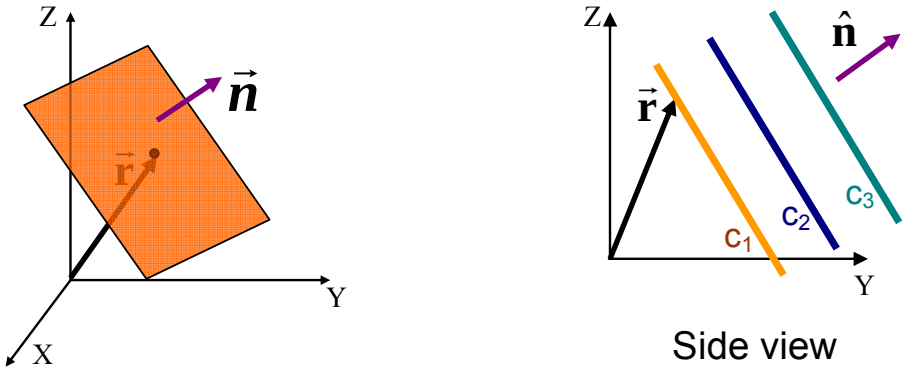


Fig. 4.5. Left: *A plane perpendicular to the unit vector* $\hat{\mathbf{n}}$. ***Right:*** *Different planes are obtained when using different values for the constant value c in the expression* $\vec{\mathbf{r}} \cdot \hat{\mathbf{n}} = c(const)$.

4.2.B Traveling Plane Waves and Phase velocity

Consider the two-variable vectorial function E of the form

$$\vec{\mathbf{E}}(\mathbf{r},t) = \vec{\mathbf{E}}_{\mathbf{o}} f\left(\underbrace{\vec{\mathbf{r}} \cdot \hat{\mathbf{n}} - \mathrm{v}t}_{phase} \right)$$

where f is an arbitrary one-variable function and $\vec{\mathbf{E}}_{\mathbf{o}}$ is a constant vector.

(For example, f could be the Cos function.)

Notice, the points over a plane oriented perpendicular to $\hat{\mathbf{n}}$ and traveling with velocity v define the locus of points where the phase of the wave $\vec{\mathbf{E}}$ remains constant. For this reason, the wave ψ is called a plane wave.

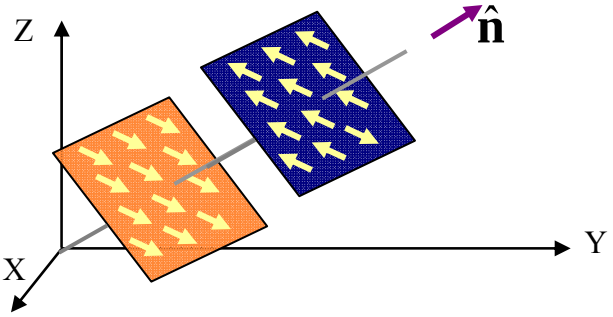


Fig. 4.6 *Schematic representation of a plane wave of electric fields. The figure shows the electric fields at two different planes, at a given instant of time. The fields lie oriented on the corresponding planes. The planes are perpendicular to the unit vector* $\hat{\mathbf{n}}$.

Traveling Plane Waves (propagation in one dimension)

$f(x - vt)$ For any arbitrary function f, this represents a wave propagating to the right with speed *v*.
f could be COS, EXP, ... etc.

$f(\underbrace{x - vt}_{phase})$ Notice, a point x advancing at speed v will keep the phase of the wave f constant.
For this reason v is called the *phase velocity* v_{ph}.

Traveling Harmonic Waves

$COS(kx - \omega t) = COS\ [k(x - \frac{\omega}{k}t)\ ]$ and $e^{i(k\,x - \omega\,t)}$

These are specific examples of waves propagating to the right with phase velocity $v_{ph} = \omega / k$.

In general $\omega = \omega\ (k)$.

Note: The specific relationship $\omega = \omega\ (k)$ depends on the specific physical system under analysis (waves in a crystalline array of atoms, light propagation in a free space, plasmons propagation at a metal-dielectric interface, etc.]

$\omega = \omega\ (k)$ implies that, for different values of k, the corresponding waves travel with different phase velocities.

4.2.C A Traveling Wave-package and its Group Velocity

Consider the expression $f(x) = (\ 1/\sqrt{2\pi}\ ) \int_{-\infty}^{\infty} F(k)\ e^{ikx} dk$ as the representation of a pulse profile at $t=0$. Here e^{-ikx} is the profile of the harmonic wave $e^{i(kx-\omega t)}$ at $t = 0$.

The profile of the pulse at a later time will be represented by,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\ e^{i(k x - \omega t)} F(k)$$

Pulse composed by a group of traveling harmonic waves (36)

Since, in the general case, each component of the group travels with its own phase velocity,

would still it possible to associate a unique velocity to the propagating group of waves?

The answer is positive; it is called *group velocity*. Below we present an example that helps to illustrate this concept.

Case: Wavepacket composed of two harmonic waves

Analytical description)

For simplicity, let's consider the case in which the packet of waves consists if only two waves of very similar wavelength and frequencies.

$$\psi(x,t) = Cos[kx - \omega t] \quad + \ Cos[\ (k + \Delta k)x - (\omega + \Delta\omega)t] \qquad (37)$$

Using the identities $Cos(A+B) = Cos(A)Cos(B) - Sin(A)Sin(B)$ and $Cos(A-B) = Cos(A)Cos(B) + Sin(A)Sin(B)$ one obtains $Cos(A+B) + Cos(A-B) = 2Cos(A)Cos(B)$, which can be expressed as $Cos(A) + Cos(B) = 2\,Cos(\frac{A+B}{2})\,Cos(\frac{A-B}{2})$

Accordingly, (38) can be expressed as,

$$\psi(x,t) = 2Cos[\ (\frac{\Delta k}{2})x - (\frac{\Delta\omega}{2})t\ ]\,Cos[\ (k+\frac{\Delta k}{2})x - (\omega+\frac{\Delta\omega}{2})t\ ]$$

Since we are assuming that $\Delta\omega << \omega$ and $\Delta k << k$, we have

$$\psi(x,t) = \underbrace{2Cos[\ (\frac{\Delta k}{2})x - (\frac{\Delta\omega}{2})t\ ]}_{\text{Modulation envelope}} Cos[\ kx - \omega t\ ] \qquad (38)$$

Notice, the modulation envelope travels with velocity equal to

$$v_g = \frac{\Delta\omega}{\Delta k}, \qquad (39)$$

which is known as the group velocity.

In summary,

$$\psi(x,t) = \underbrace{2Cos[\ (\frac{\Delta k}{2})x - (\frac{\Delta\omega}{2})t\ ]}_{\textbf{Amplitude Modulating wave}}\ \underbrace{Cos[\ kx - \omega t\ ]}_{\textbf{Carrier wave}} \qquad (40)$$

Planes where the ***amplitude of the resultant wave remains constant*** *travel with speed* $V_g = \frac{\Delta\omega}{\Delta k}$

Plane of ***constant phase*** *traveling with speed* $V_p = \frac{\omega}{k}$

The *phase velocity* is a measure of the velocity of the harmonic waves components that constitute the wave.

The *group velocity* is the velocity with which, in particular, the profiles of maximum interference propagate.
More general, the *group velocity* is the velocity at which the "envelope" profile propagate (as will be observed better in the graphic analysis given below).

Graphical description

- **EXAMPLE-1:** Visualization of the addition of two waves whos k's and ω's are very similar in value.

  Let,

$$C(z, t) = \text{Cos}\,[k_1 z - \omega_1 t] = \text{Cos}\,[\,2\,z - 5\,t\,] \qquad (41)$$

$$D(z, t) = \text{Cos}\,[k_2 z - \omega_2 t] = \text{Cos}\,[\,2.1\,z - 5.25\,t\,]$$

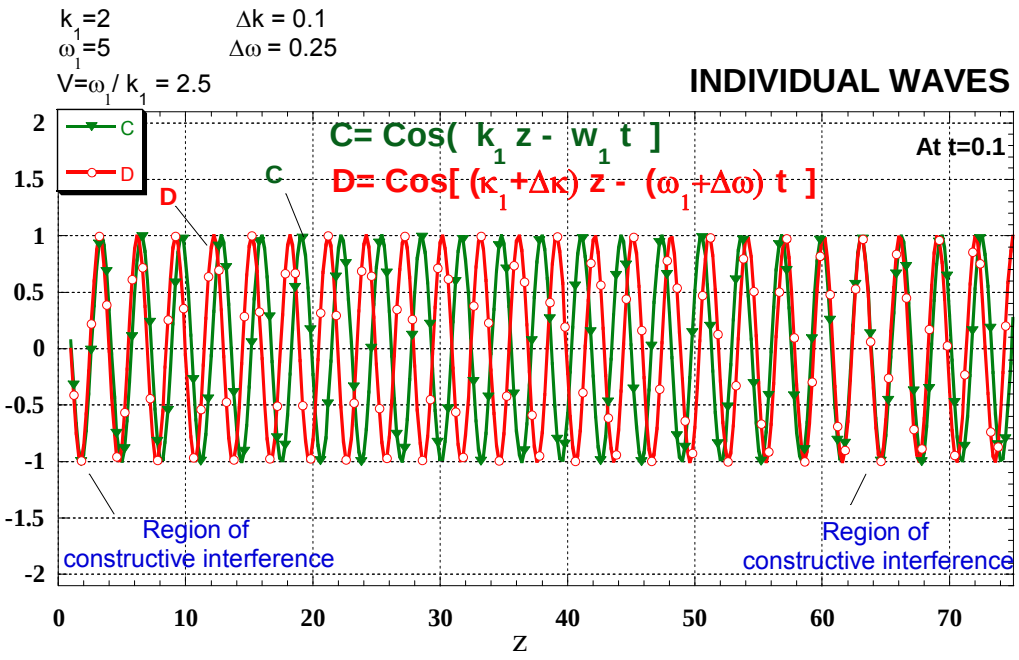


Fig. 4.7a The profile of the individual waves C(z, t) and D(z, t) are plotted individually at t= 0.1 over the 0<z<75 range.

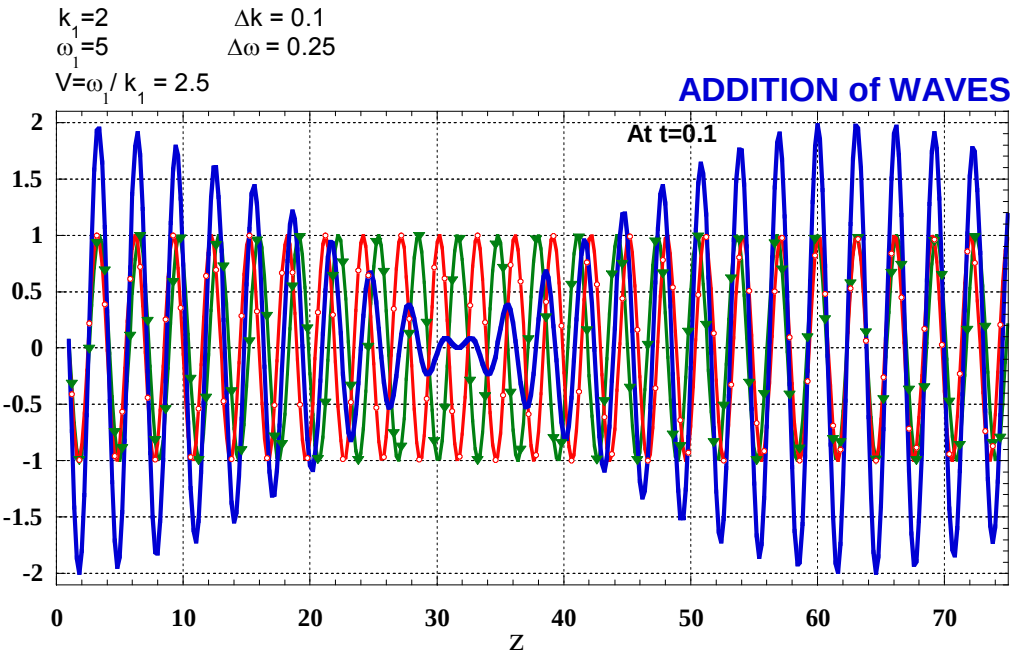


Fig. 4.7b The profile of the individual waves C(z, t) and D(z, t) as well as the profile of the sum C(z, t) + D(z, t) are plotted at t= 0.1 over the 0<z<75 range

The two plots given above are repeated once more but over a larger range in order to observe the multiple regions of constructive and destructive interference.

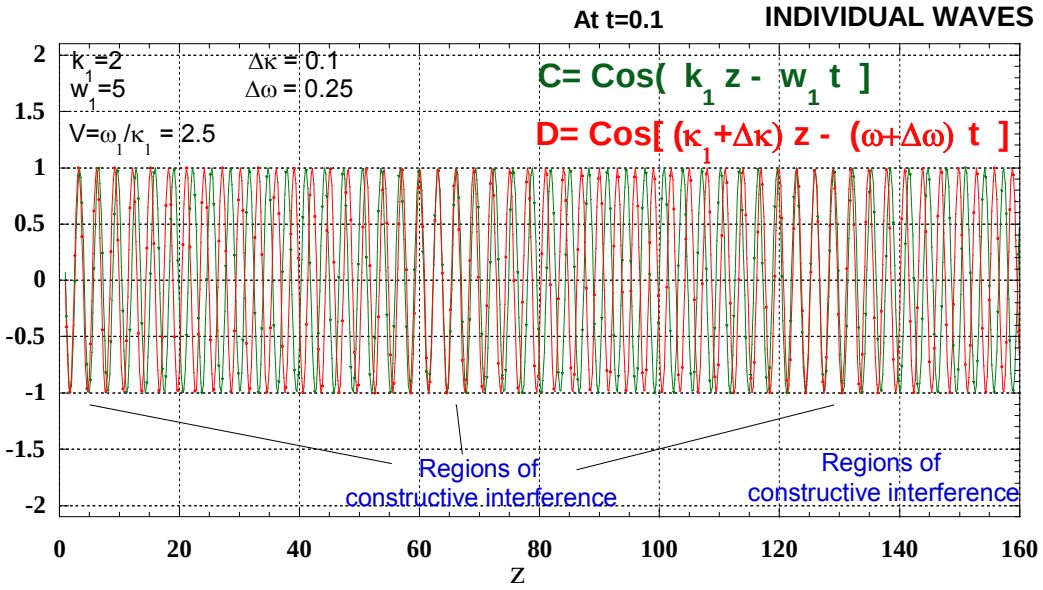


Fig. 4.8a

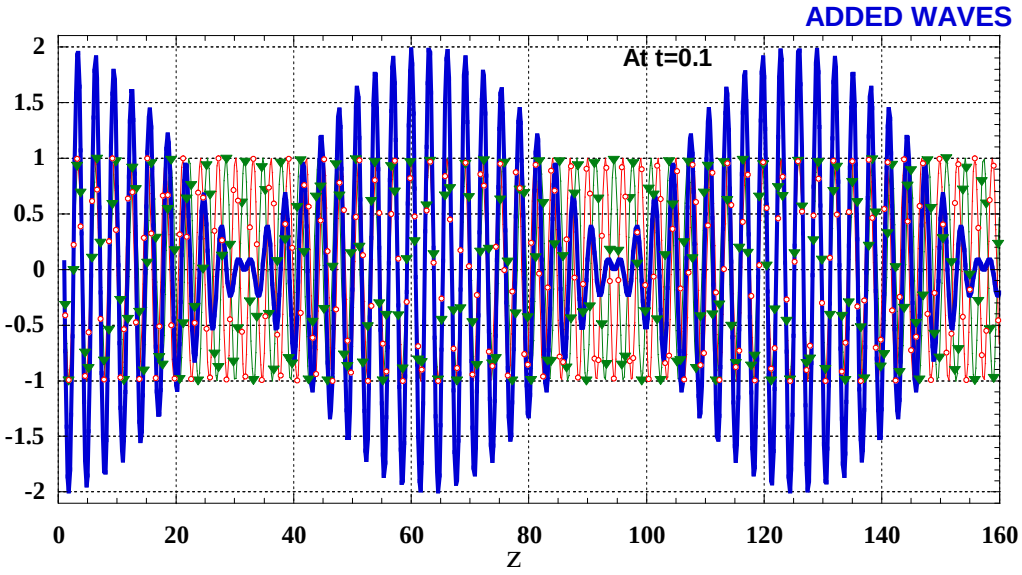


Fig. 4.8b The profile of the individual waves C(z, t) and D(z, t) given in expression (41) above, as well as the profile of the sum C(z, t) + D(z, t) are plotted at t= 0.1 over the 0<z<160 range

The wave C(z, t) + D(z, t) (the individual waves given in expression (41) above) is plotted at 2 different times in order to observe to observe the net motion of the interference profiles (group velocity).

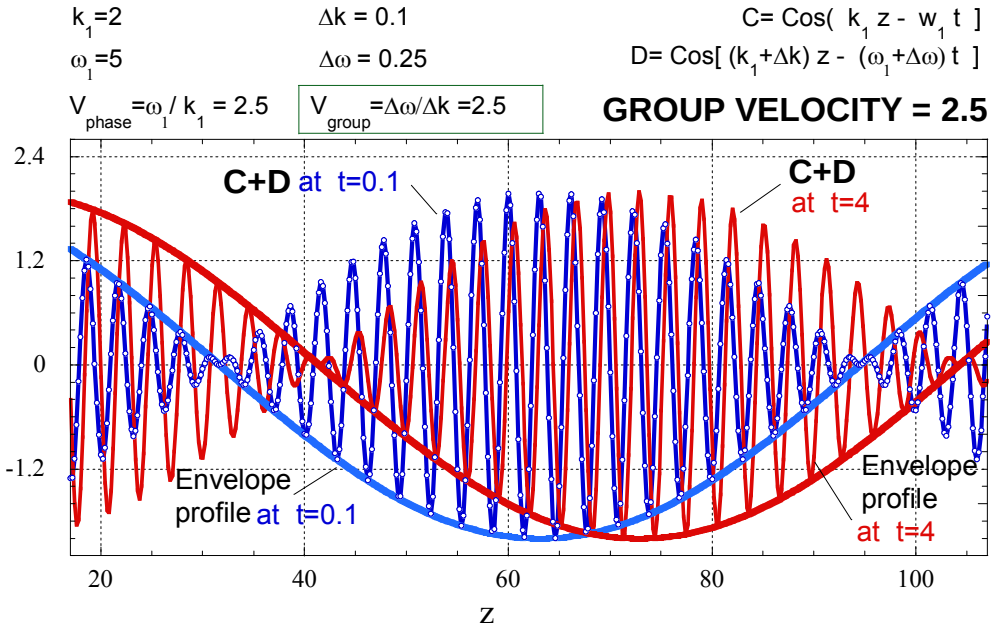


Fig. 4.9 Verify by yourself, measuring in the graph above that the net displacement of the valley (~10) divided by the incremental time (4-0.1=3.9), that the envelope profile travels with a velocity equal to 10/3.9 ~ 2.5. This value coincides with $\Delta\omega/\ \Delta k$ = 0.25/01.

In the example above:

Phase velocity of the individual waves is 2.5

Group velocity is 2.5

- **EXAMPLE-2:** Visualization of the addition of two waves whos k's and ω's are very similar in value.

  Let,

$$C(z, t) = \text{Cos}\,[k_1 z - \omega_1 t] \;=\; \text{Cos}\,[\,2\,z - 5\,t\,] \qquad (42)$$

$$D(z, t) = \text{Cos}\,[k_2 z - \omega_2 t] \;=\; \text{Cos}\,[\,2.1\,z - 5.1\,t\,]$$

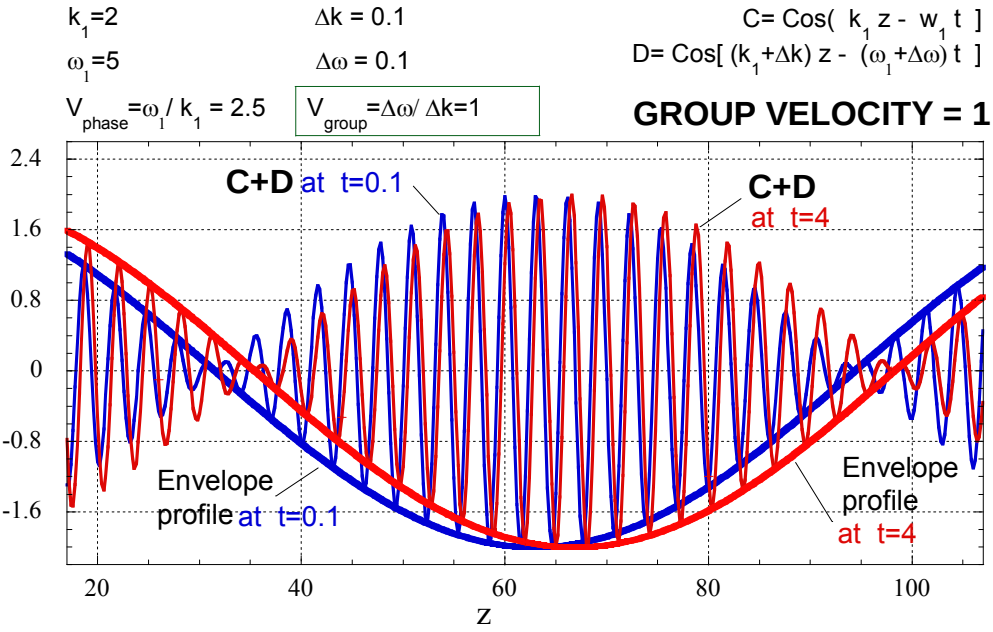


Fig. 4.10 Verify by yourself, measuring in the graph above that the net displacement of the valley (~4) divided by the incremental

time (4-0.1=3.9), that the envelope profile travels with a velocity equal to 5/3.9 ~ 1. This value coincides with $\Delta\omega/\Delta k$ = 0.1/01.

In the example above:

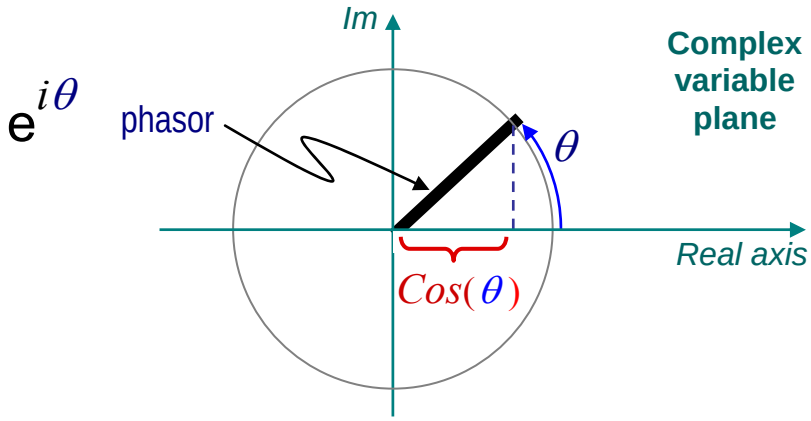
Phase velocity of the individual waves is 2.5

Group velocity is 2.5

Comparing Fig. 4.9 and Fig. 4.10 we get evidence that the wavepackets of the higher group velocity advances more than the one lower group velocity, despite the fact that the components have similar phase velocity..

Phasor method to analyze a wavepacket

It becomes clear from the analysis above that a packet composed of only two single harmonic waves of different wavelength can hardly represents a localized pulse. Rather, it represents a train of pulses. Let's try to understand qualitatively (using the method of phasors) the reasons for the formation of a train of pulses.



$\theta = kx-\omega t$

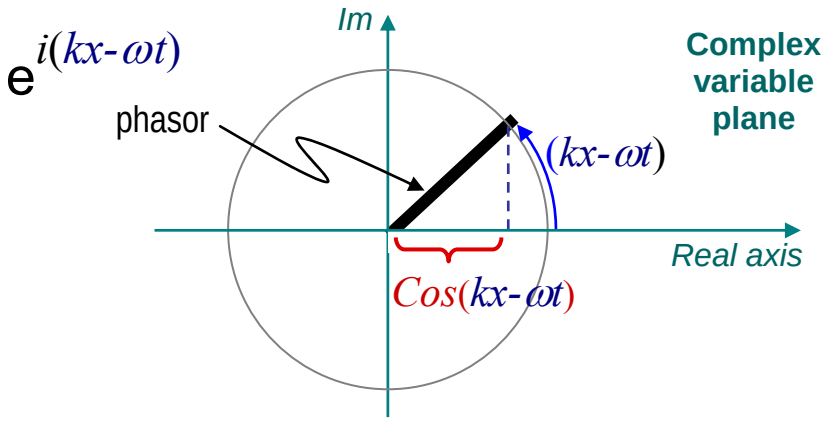
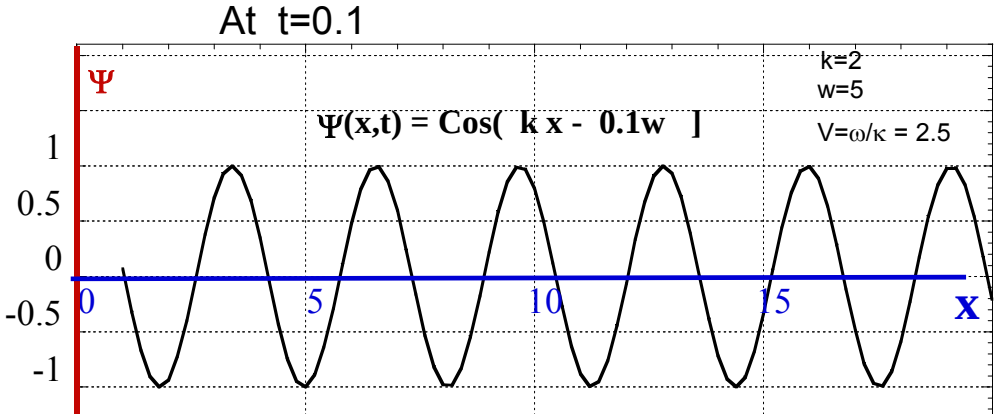
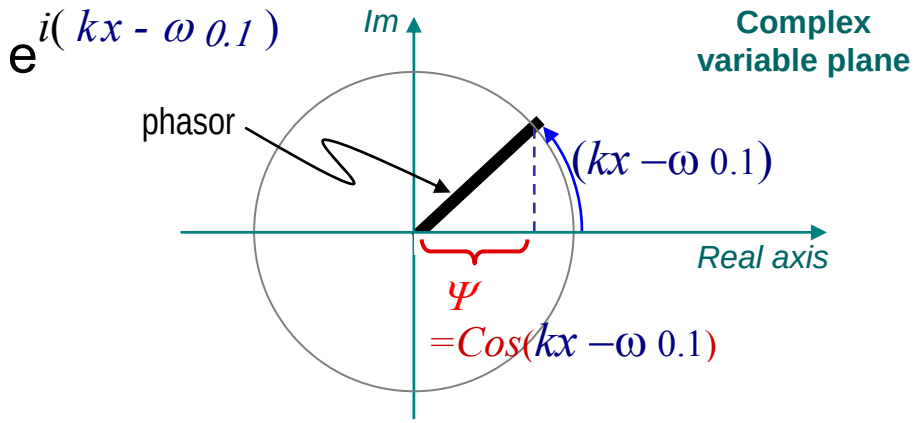


Fig. 4.10 *A phasor representation in the complex plane.*

Analysis at a given fixed time (t= 0.1)





Analysis at a given fixed position (x= 5)
(Assignment)

Case: wavepacket composed of two waves

Let's consider the addition of two harmonic waves

$$Cos(\underbrace{k_A x}_{phase}) + Cos(\underbrace{k_B x}_{phase}) \qquad (42)$$

where $k_A < k_B$, and $k_B - k_A \equiv \Delta k$.

To evaluate (42) we will work in the complex plane. Accordingly, to each wave we will associate a corresponding phasor,

$$e^{ik_A x} + e^{ik_B x}$$

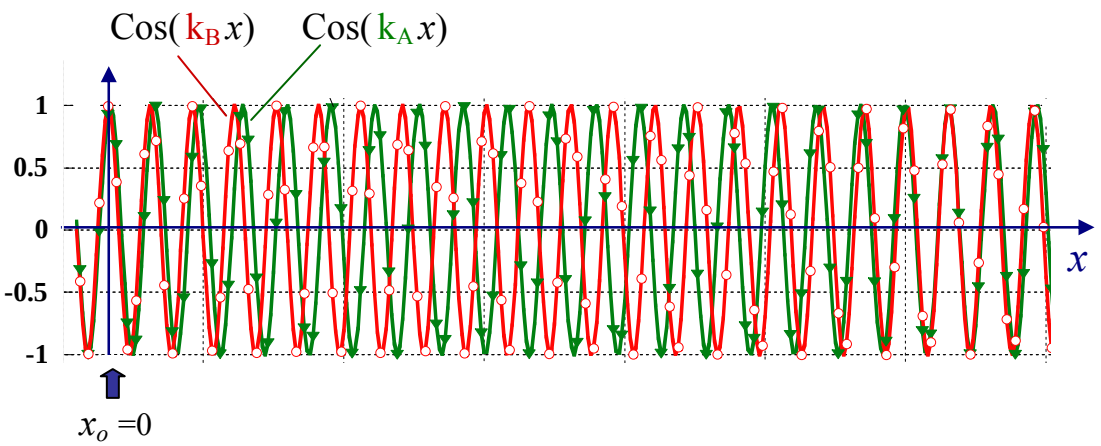
The projection of the (complex) phasors along the horizontal axis gives the real-value we are looking for in (42).

At a given position x, the phase-difference between the two wave profiles is equal to,

$$\textit{Phase difference} = k_B x - k_A x = (k_B - k_A)x \qquad (43)$$

The following happens:

a) The waves interfere constructively at $x = 0 \equiv x_o$ (both waves have a phase equal to zero.)



b) As x increases a bit, the interference is not as perfect since the phase of the waves start to differentiate from each other $(k_B - k_A)x \neq 0$; consequently the sum of the waves should display an oscillatory behavior as x increases.

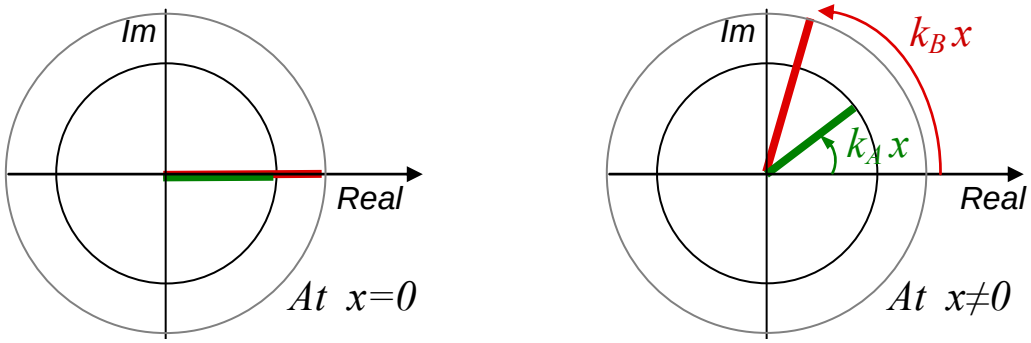


Fig. 4.11 *Analysis of wave addition by phasors in the complex plane. For clarity, the magnitude of one of the phasors has been drawn larger than the other one.*

c) As x increases, it will reach a particular value $x = x_1$ that makes the phase difference between the waves equal to 2π. The value of x_1 is determined by the condition,

$$(k_B - k_A)x_1 = 2\pi$$

That is, the waves interfere constructively again at $x_1 = 2\pi / \Delta k$, where $k_B - k_A \equiv \Delta k$

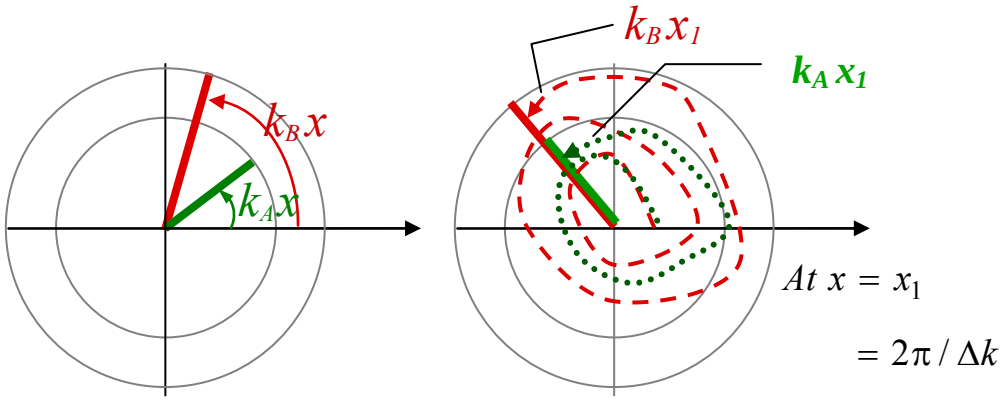
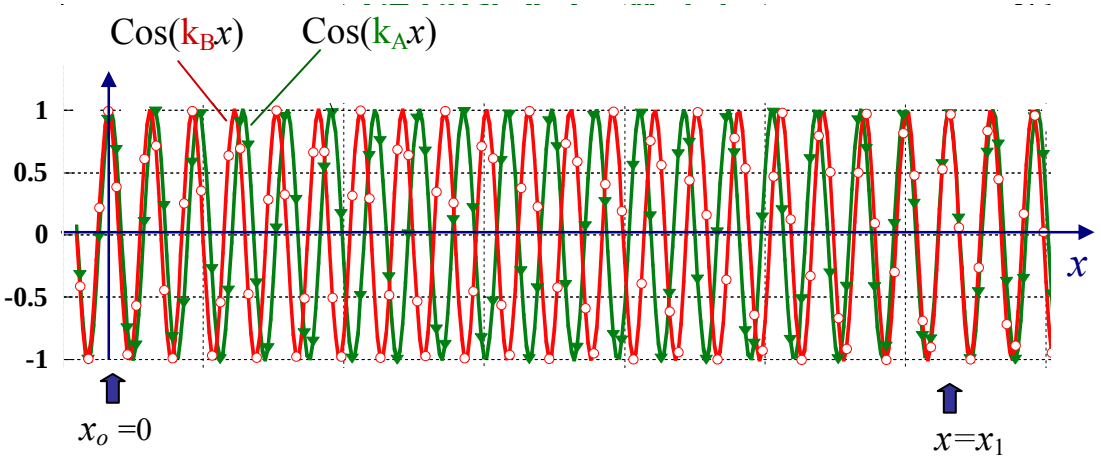


Fig. 4.12 Left: In general the phasors do not coincide. **Right:** At a specific value of x=x_1, both phasors coincide, thus giving a maximum value to the sum of the waves (at that location.) The phasors diagram also makes clear that as x keeps increasing, constructive interference will also occur at multiple values of x_1.

It is expected then that the wave-pattern (the sum of the two waves) observed around $x = 0$ will repeat again at around $x = x_1$.



d) Notice that additional regions of constructive interference will occur at positions $x = x_n$ satisfying $(k_B - k_A)x_n = n\ 2\pi$ or $x_n = n\ 2\pi / \Delta k$ ($n = 1, 2, 3, \ldots$) The phasors diagram, therefore, makes clear that as x keeps increasing, additional discrete values (x_1, x_2, x_3, etc) will be found to produce additional maxima.

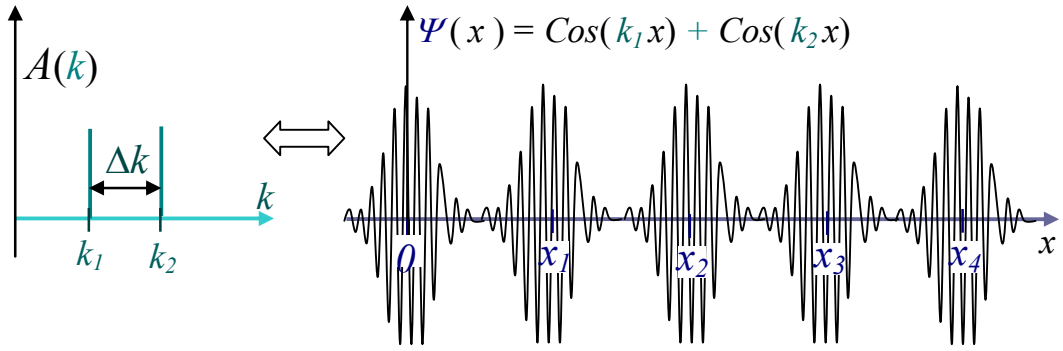


Fig. 4.13 Wavepacket composed of two harmonic waves

Case: A wavepacket composed of several harmonic waves

When adding several harmonic waves $\sum_{i=1}^{M} A_i Cos(k_i x\ )$, with M >2, the condition for having repeated regions of constructive interference still can occurs. In effect,

- First, there will be of course a constructive interference around x=0.
- Second, we expect the existence of a position $x=x_1$ that will make each of the quantities $(k_i\text{-}k_j)x_1$ equal to a multiple of 2π.

  $(k_i\text{-}k_j)x_1$ = (integer)$_{ij}$ 2π (44)

  (for all the ij combinations, with i and j = 1, 2, 3, … , M).

  When this happens, it would mean that all the corresponding phasors coincide, thus giving a maximum of amplitude.
- Third, additional regions of maximum interference will occur at multiple integers of x_1.

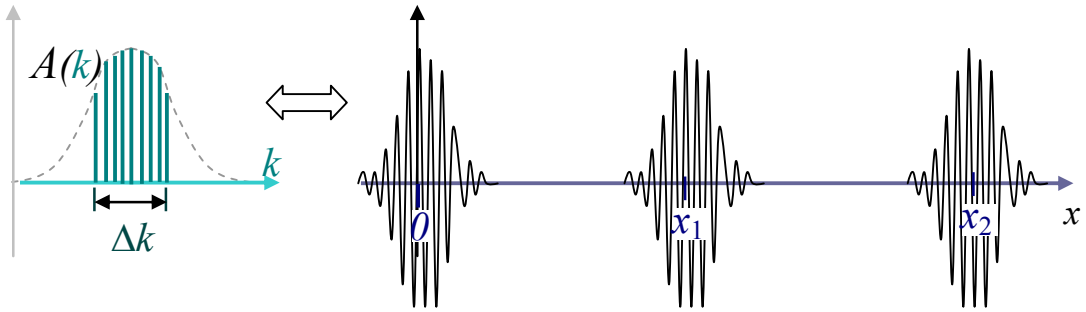


Fig. 4.14 *Wavepacket composed of a large number of harmonic waves (to be compared with Fig. 4.13 above.) The train of pulses are more separated from each other.*

Notice also that,

the greater the number M of harmonic components in the packet (with wavevectors k_i within the same range Δk shown in the figure above),

the more stringent becomes for all the M waves to satisfy at once the condition (44) for constructive interference.

This means, a greater value of x may be needed any time an extra number of harmonic waves are included in the packet.

Since the other maxima of interference occur at multiple values of x_1, we expect, therefore, that the greater number of k-values (within the same range Δk), the more separated from each other will be the regions of constructive interference. This is shown in Fig. 4.14.

Case: Wavepacket composed of an infinite number of harmonic waves

Adding more and more wavevectors k (still all of them within the same range Δk show in the figure below)) will make the value of x_1 to become greater and greater. As we consider a continuum variation of k, the value of x_1 will become infinite. That is, we will obtain just one pulse.

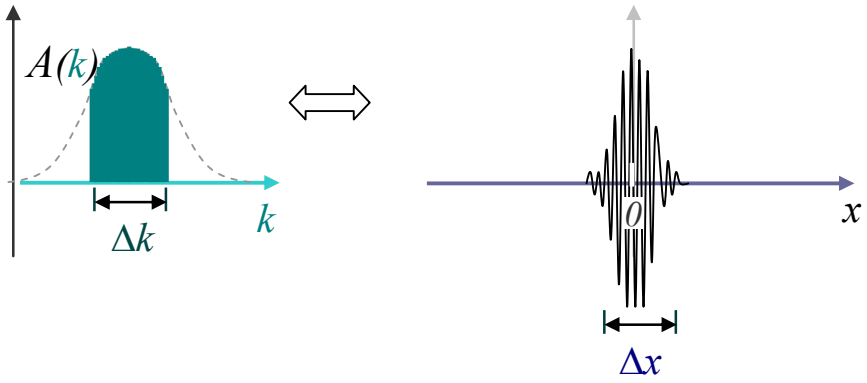


Fig. 4.15 *Wavepacket composed of wavevectors k within a continuum range Δk produces a single pulse.*

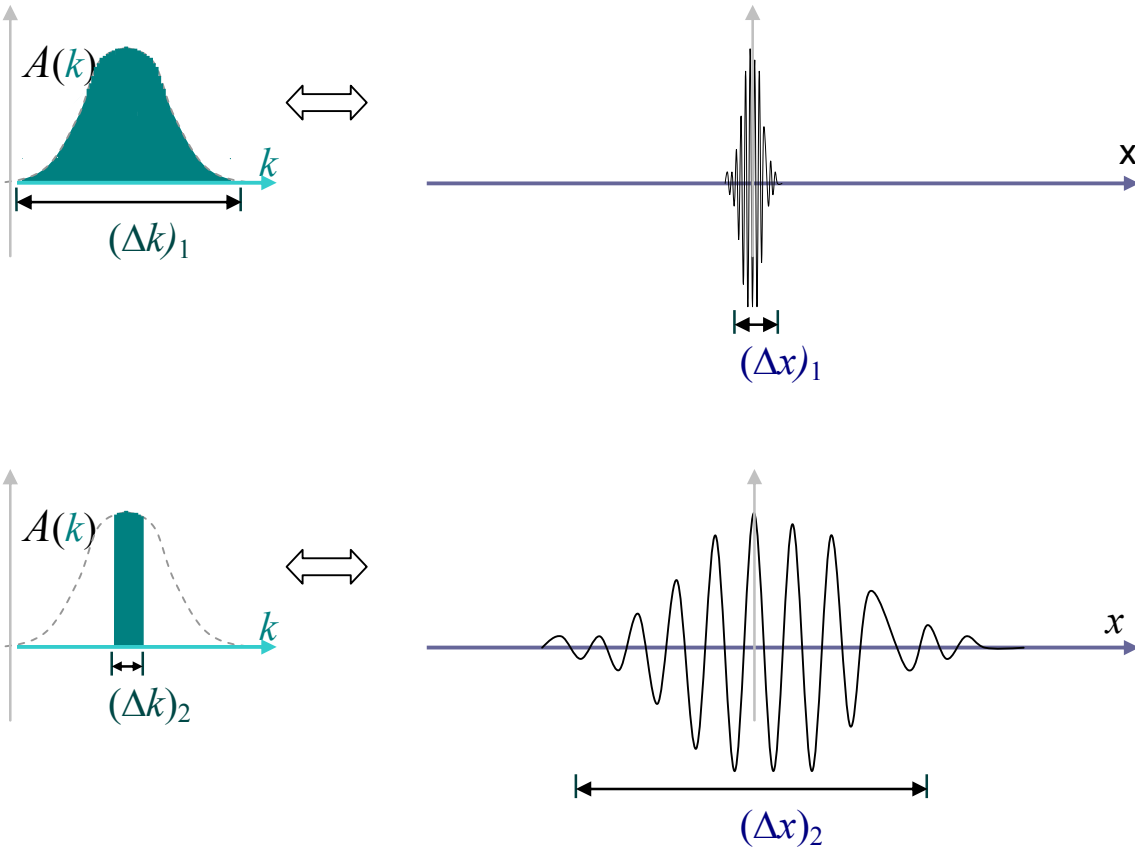
What a bout the variation of the pulse-size as the number of wavevectors (all with values within the range Δk) increases?

Fig. 4.15 above already suggests that the size should decrease. In effect, as the number of harmonic waves increases, the multiple addition of waves tends to average out to zero, unless x =0 or for values of x very small; that is the pulse becomes narrower.

Thus, we now can understand better the property stated in a previous paragraphs above (see expression (29) above, where the properties of the Fourier transform were being discussed.)

the more localized the function the broader its spectral response; and vice versa.

In effect, notice in the previous figure that if we were to increase the range Δk , the corresponding range Δx of values of the x coordinate for which all the harmonic wave component can approximately interfere constructively would be reduced; and vice versa.



In short:

$$\Delta x \sim \frac{1}{\Delta k} \tag{45}$$

This is a general property of the Fourier analysis of waves (in principle, it has nothing to do with Quantum Mechanics.

We will see later that one way to describe QM is within the framework of Fourier analysis. In this context, some of the mathematical terms are identified (via the de Broglie hypothesis) with the particle's physical variables, which, accordingly, become subjected to the relationship indicated in (45). The realization that physical variables are subjected to the relationship (45) constitutes one of the cornerstones of Quantum Mechanics. We will explore this concept in the following sections.

4.3 DESCRIPTION of a FREE PARTICLE MOTION

According to Louis de Broglie, a particle of linear momentum p and total energy E is associated with a wavelength an a frequency given by,

$\lambda = h / p$ where λ is the wavelength of the wave associated with the particle's motion; and

$\gamma = E / h$ the total energy E is related to the frequency v of the wave associated with its motion.

where h is the Planck's constant; h =6.6x10^{-34} *Js*.

But the de Broglie postulate does not tell us how the wave-particle propagates.
If, for example, the particle were to be subjected to forces, its momentum could change in a very complicate way, and potentially not a single wavelength would be associated to the particle (maybe many harmonic waves would be needed to localize the particle.) The de Broglie postulate does not allow predicting such dynamic response (the Schrodinger equation, to be introduced in subsequent chapters, does that.)

As a first attempt to describe the propagation of a particle (through the space and time) lets consider first the simple case of a free particle (free particle motion implies that its momentum p and energy E remain constant.) Our task is to figure out the wavefunction that describes the free motion of the particle.

4.3.A Proposition-1: Using a wavefunction with a definite linear momentum

- Taking into account the associated de Broglie's wavelength λ and frequency ν, let's construct (by making an arbitrary guess) a wavefunction of the form,[1]

$$\left.\begin{aligned}\psi(x,t) &= ACos\,[\frac{2\pi}{\lambda}x - 2\pi\ vt] \\ &\quad math \\ &= ACos\,[\frac{2\pi}{h}(px - Et)] \\ &\quad physics\end{aligned}\right\}$$ *First attempt to describe a free-particle wave-function* (46)

Once we make this connection, the physics will be bounded by whatever mathematical properties the waves $Cos\,[\frac{2\pi}{\lambda}x - 2\pi\ vt]$ have.

Notice in (46) that, in this particular case a single value of linear momentum characterizes this function; that is p.

- This (guessed) wavefunction (46) is proposed following an analogy to the description of electromagnetic waves,

$$\mathcal{E}(x,t) = \mathcal{E}_o Cos\,[\frac{2\pi}{\lambda}x - vt] \qquad \textit{electric field wave} \qquad (47)$$

where, as we know, the intensity I (energy per unit time crossing a unit cross-section area perpendicular to the direction of radiation propagation) is proportional to $|\mathcal{E}(x,t)|^2$.

- Let's check whether or not the proposed wavefunction (46) is compatible with our classical observations of a free particle motion. For example, if our particle were moving with a classical velocity v_0, would we get the same value (somehow) from the wavefunction (46)?
First, notice for example that this wavefunction has a phase velocity given by,

$$v_{wavefunction} = E/p \qquad \textit{(phase velocity)} \qquad (48)$$

In the non relativistic case, if we used in (48) the classical values

$$E = \frac{1}{2}m(v_{classical})^2, \text{ and } p = mv_{classical},$$

we would obtain from (48),

$$v_{wavefunction} = \frac{1}{2} v_{classical} \tag{49}$$

We realize here a disconnection between the waveparticle description (the wave described by expression (46) travels with speed $v_{classical}/2$) and the expected result is to have a particle that moves with speed $v_{classical}$).

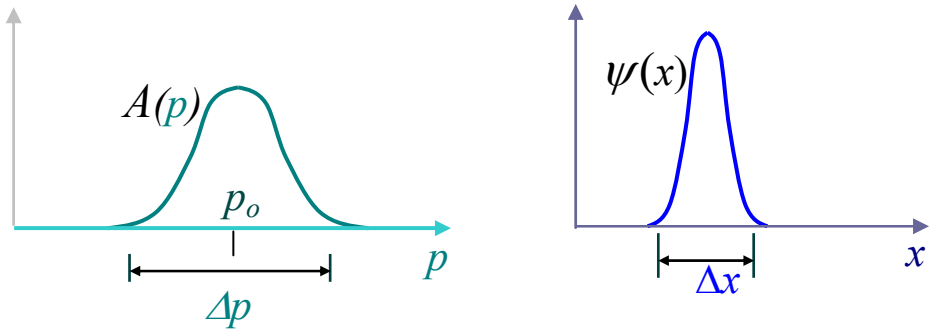
This apparent shortcoming may be attributed to the fact that, in the classical view, a particle occupies a finite region of the space, while the wavefunction proposed in (46) has an infinite spatial extension. Apparently, a better option would be to select a wavepacket in order to describe a more localized function. Let's explore this idea.

4.3.B Proposition-2: Using a wavepacket as a wavefunction

Let's assume our classical particle of mass m is moving with velocity

$$v_{classical} = v_o \tag{50}$$

(or approximately equal to v_o). Accordingly, let's build a wavepacket whose dominant harmonic component is the one with wavelength $\lambda_o = h/mv_o$ (or, equivalently, in terms of the variable $p = h/\lambda$) a packet whose dominant harmonic component is the one with $p = p_o = mv_o$



$$\psi(x,t) \sim \int_{\Delta\lambda} A Cos\ [\frac{2\pi}{\lambda} x - 2\pi\ vt]\ d\lambda$$

In terms of the momentum variable $p = h/\lambda$

$$\psi(x,t) \sim \int_{\Delta p} A(p) Cos\ [\frac{2\pi}{h}(px - Et)]\ dp$$

where $E = E(p) = p^2/2m$ (we are considering a free and no relativistic particle)

Using the variables

$$k \equiv \frac{2\pi}{h} p \quad \text{and} \quad \omega \equiv \frac{2\pi}{h} E\ , \tag{51}$$

and expressing the package rather with the complex variable, we propose

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\Delta k} A(k) e^{i[(kx - \omega t)]}\ dk \tag{52}$$

For a free particle (in the non relativistic case) $E = \frac{p^2}{2m}$. Thus, since ω depends on E, and E depends on p we have ω = ω (*k*). Indeed,

$$\omega(k) = \frac{2\pi}{h} E = \frac{2\pi}{h} \frac{p^2}{2m} = \frac{h}{2\pi} \frac{k^2}{2m}$$

The group velocity of the wave-packet is given by,

$$\mathrm{v}_{\substack{wavefunction's \\ group\text{-}vellocity}} = \left.\frac{d\omega}{dk}\right|_{k_o} = \frac{h}{2\pi} \frac{k_o}{m} \tag{53}$$

According to (51), $k_o \equiv \frac{2\pi}{h} p_o = \frac{2\pi}{h} m\ \mathrm{v}_o$

$$\mathrm{v}_{\substack{wave\text{-}function's \\ group\text{-}vellocity}} = \left.\frac{d\omega}{dk}\right|_{k_o} = \frac{p_o}{m} = \mathrm{v}_o = \mathrm{v}_{classical} \tag{54}$$

Thus, it is the group velocity of the wave-packet what represents the velocity of the particle.

Consequences:

Notice, if a wave-packet (composed of harmonic wave with p-values within a given range Δp) is going to represent a particle, then a pulse of corresponding extension Δx will be interpreted as the particle's position. That is, there is not a definite exact position to be associated with the particle, but rather a range of possible values (within Δx.)That is, there is an uncertainty in the particle's position.

In addition, if the Fourier analysis is providing the right tool to make connections between the wave-mechanics and the expected classical results (for example, it allow us to identify the classical velocity with the wave-packet's group velocity) then we should be bounded by the other consequences inherent in the Fourier analysis. One of them, for example, is that $\Delta x \sim \frac{1}{\Delta k}$ (see statement (29) and expression (45) above), which has profound consequences in our view of the mechanics governing Nature.

Indeed, from (51) $\Delta k \equiv \frac{2\pi}{h}\Delta p$; thus $\Delta x \sim \frac{1}{\Delta k}$ implies $\Delta x \sim \frac{1}{\frac{2\pi}{h}\Delta p} = \frac{\hbar}{\Delta p}$,

where we have defined $\hbar \equiv h/2\pi$.

$\Delta x \sim \hbar / \Delta p$ implies that the better we know the momentum of the particle (that is, the narrower the range Δp in the wave-packet), the larger uncertainty Δx to locate the particle. (55)

This is quite an unusual result to classical mechanics, where we are used to specify the initial conditions of a particle's motion by giving the initial position and initial velocity *simultaneously* with limitless accuracy. That is, we are used to have Δx and Δp specified as narrow as we want (we assume there was nothing wrong with it.) By contrary, in the world where the dual wave-particle reins, we have to live with the constrain that (55) implies: we can not improve the accuracy in knowing Δx without scarifying the accuracy of Δp, and vice versa. In the next chapter we will further familiarize with this new quantum behavior.

[1] Here we follow closely Quantum Physics, Eisberg and Resnick, Section 3.2