CHAPTER-5  WAVEPACKETS and THE HEISENBERG UNCERTAINTY PRINCIPLE

Fourier Spectral Decomposition of the Wave-function

Understanding of the Heisenberg Uncertainty Principle (as a universal properties of waves)

Describing the wavefunction of a free-particle (relativistic and non-relativistic cases) in the context of the wave-particle duality

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CHAPTER-5  WAVEPACKETS and THE HEISENBERG UNCERTAINTY PRINCIPLE

Objective: The develop the concepts of “group velocity of a wavepacket,” and the “inner product” between functions (cases of real and complex functions) in order to gain a plausible understanding of the Heisenberg Uncertainty Principle. The wavepacket is decomposed in term of its Fourier components. The inner product is expressed in regular as well as in bracket notation. A quantum mechanics description of the free particle for the non-relativistic and relativist cases are obtained.

In an effort to reach a better understanding of the wave-particle duality\(^1\), the motion of a free-particle will be described by a wave packet \(\Psi = \Psi(x,t)\) composed of traveling harmonic waves,

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

A wavepacket is a function whose values, at a given time, are different from zero only inside a limited spatial region of extension \(\sim \Delta X\). From a quantum mechanics point of view, if a wavepacket of width \(\Delta X\) is used to represent a particle, \(\Delta X\) is then interpreted as the region where the particle is likely to be located; that is, there is an uncertainty about its “exact” location. There will be also an uncertainty \(\Delta P\) about the linear momentum of that particle. In this chapter we try to understand how these two uncertainties, \(\Delta X\) and \(\Delta P\), do relate to each other. Of course, we know those uncertainties are related through the quantum Heisenberg Principle, but we plan to provide some arguments of why such quantum principle should follow.

**STRATEGY:**
First, we summarize some general properties of waves and use the Fourier’s spectral decomposition technique as the analytical tool to describe wavepackets.

Then, when the De Broglie’s principle of wave-particle duality is integrated into this description, the interrelation between the spatial and momentum...
uncertainties, the Heisenberg Principle, will fit in a very logical and consistent way.

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

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

However, it should be mentioned that such a Fourier analysis is a particular case of a broader mathematical approach that describes a given function $\Psi$ as a linear combination of a well-defined set of functions, which are referred to as a basis.

basis-functions \{ $\varphi_1$, $\varphi_2$, $\varphi_3$, ... \}.

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.

5.1.A Analogy between the components of a vector “$v$” and the spectral components of a function “$\Psi$”

Let’s consider the analogy between the components of a three dimensional vector, and the spectral decomposition of an arbitrary function $\Psi$. 
Vector components
In the expression (1) above,
\[
\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}
\]
is a set of unit vectors perpendicular to each other; that is,
\[
\hat{e}_i \cdot \hat{e}_j = \delta_{ij}
\]
where \(\delta_{ij} \equiv 0\) if \(j \neq i\)
\(\equiv 1\) if \(j = i\) (3)

Here \(A \cdot B\) means "scalar product between vector \(A\) and vector \(B\)."

How to find the components of a vector \(v\) ?
- If, for example a vector \(v\) were expressed as
\[ \mathbf{v} = 3 \hat{e}_1 + 7 \hat{e}_2 - 2 \hat{e}_3, \]
then, its component would be given by
\[ \hat{e}_1 \cdot \mathbf{v} = 3; \quad \hat{e}_2 \cdot \mathbf{v} = 7; \quad \text{and} \quad \hat{e}_3 \cdot \mathbf{v} = -2 \]

- In a more general case,

\[ \text{if } \mathbf{v} = v_1 \hat{e}_1 + v_2 \hat{e}_2 + v_3 \hat{e}_3 \]
its components \( v_j \) are obtained by evaluating the corresponding scalar products
\[ v_j = \hat{e}_j \cdot \mathbf{v}; \quad \text{for } j=1,2,3 \]

Thus, a vector \( \mathbf{v} \) can be expressed in terms of the unit vectors in a compact form,
\[ \mathbf{v} = \sum_{j=1}^{3} (\hat{e}_j \cdot \mathbf{v}) \hat{e}_j \]
(4)

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

5.1. 

**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, they fulfill the following relation,
\[ \varphi_i \cdot \varphi_j = \delta_{ij} \]

But what would the symbol \( \cdot \) mean?

To answer this question, we will introduce a definition. **Let’s consider first** the particular case where all the functions under consideration are periodic and real.

Let \( \lambda \) be the periodicity of the functions; that is,
\[ \Psi(x + \lambda) = \Psi(x) \]
(6)

**Definition.** A scalar product between two periodic (but otherwise arbitrary) real functions \( \Psi \) and \( \Phi \) is defined as follows,
\[ \psi \cdot \phi \equiv \int_0^\lambda \psi(x) \Phi(x)dx \]

(Throughout these lecture notes, the symbol “≡” means “definition”).

Rather than using \( \Psi \cdot \Phi \), a more common notation is \( (\psi, \phi) \)

\[
(\psi, \phi) \equiv \int_0^\lambda \psi(x) \Phi(x)dx \quad \text{definition of “scalar product” for the case of real functions} \tag{7}
\]

In Section 5.1.F below, we extend this definition to include functions whose values lie in the complex variable domain.

Note: Notice the similarity between the scalar product of two vectors and the scalar product of two functions

\[
v = v_1 \hat{e}_1 + v_2 \hat{e}_2 + v_3 \hat{e}_3 \quad \Psi: \quad \ldots \Psi(x_1) + \Psi(x_2) + \Psi(x_3) + \Psi(x_4) + \ldots
\]

\[
w = w_1 \hat{e}_1 + w_2 \hat{e}_2 + w_3 \hat{e}_3 \quad \Phi: \quad \ldots \phi(x_1) + \phi(x_2) + \phi(x_3) + \phi(x_4) + \ldots
\]

\[
v \cdot w = v_1 w_1 + v_2 w_2 + v_3 w_3 \quad (\psi, \phi) = \ldots + \Psi(x_1)\phi(x_1) + \Psi(x_2)\phi(x_2) + \Psi(x_3)\phi(x_3) + \ldots
\]

**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,

\[
(\varphi_i, \varphi_j) \equiv \int_0^\lambda \varphi_i(x)\varphi_j(x)dx = \delta_{ij} \tag{8}
\]

**Exercise:** Given the functions \( \varphi \) and \( \psi \),

\[
\varphi(x) = \cos(x) \quad \text{and} \quad \psi(x) = \sin(x), \quad \text{defined over the range } (0, 2\pi),
\]

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

\[
\langle \psi | \Phi \rangle \text{ instead of } (\psi, \Phi)
\]

Although 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 also 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 literature, we will frequently use it in this course.

5.1.C How to find the spectral components of a function $\Psi$?

Given an arbitrary periodic function $\Psi$ we wish to express it as a linear combination of a given base of orthogonal periodic functions $\{ \varphi_j, j=1, 2, \ldots \}$

$$\Psi = c_1 \varphi_1 + c_2 \varphi_2 + \ldots$$

(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),

$$c_j = \langle \varphi_j | \psi \rangle = \int_0^\lambda \varphi_j(x) \psi(x) dx \quad \text{for } j=1,2,3, \ldots$$

(10)

Still one question remains: How do the functions $\varphi_j$ look like?

Answer:

- There exist different types of basis 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 9).

- One particular basis set is the one composed by harmonic functions

  BASE SET $\{ \cos_0, \cos_1, \sin_1, \cos_2, \sin_2, \ldots \}$

  where

  $$\cos_0(x) \equiv \sqrt{\frac{1}{\lambda}}; \quad \cos_n(x) \equiv \sqrt{\frac{2}{\lambda}} \cos\left(\frac{2\pi}{\lambda} \frac{x}{n}\right); \quad \text{for } n = 1, 2, \ldots$$

  (11)

  $$\sin_n(x) \equiv \sqrt{\frac{2}{\lambda}} \sin\left(\frac{2\pi}{\lambda} \frac{x}{n}\right); \quad \text{for } n = 1, 2, \ldots$$

which are useful to describe any periodic function $\Psi$ of period equal to $\lambda$. 


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

\[ < \cos_n | \sin_m > = \int_0^\lambda \cos_n(x) \sin_m(x) dx = 0 \]

More generally,

\[
\begin{align*}
< \cos_n | \sin_m > &= 0 & \text{for arbitrary integers } m, n; \\
< \cos_n | \cos_m > &= \delta_{nm} & \text{for arbitrary integers } m, n; \\
< \sin_n | \sin_m > &= \delta_{nm} & \text{for arbitrary integers } m, n.
\end{align*}
\]  

(12)

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

The property (12) leads to the following result:

Using the base-set of harmonic functions of periodicity \( \lambda \), defined as follow,
\{ \text{Cos}_o, \text{Cos}_1, \text{Sin}_1, \text{Cos}_2, \text{Sin}_2, \ldots \}\]

where

\[
\text{Cos}_o(x) \equiv \frac{1}{\sqrt{\lambda}},
\]

\[
\text{Cos}_n(x) \equiv \frac{1}{\sqrt{\lambda}} \cos\left(\frac{2\pi}{\lambda/x} x\right) \quad \text{for} \ n = 1, 2, \ldots;
\]

\[
\text{Sin}_n(x) \equiv \frac{1}{\sqrt{\lambda}} \sin\left(\frac{2\pi}{\lambda/x} x\right) \quad \text{for} \ n = 1, 2, \ldots.
\]

the following theorem results:

An arbitrary function \( \Psi' \) of period \( \lambda \) can be expressed as,

\[
\Psi'(x) = A_o \text{Cos}_o(x) + \sum_{n=1}^{\infty} A_n \text{Cos}_n(x) + \sum_{n=1}^{\infty} B_n \text{Sin}_n(x)
\]

or simply

\[
\Psi' = A_o \text{Cos}_o + \sum_{n=1}^{\infty} A_n \text{Cos}_n + \sum_{n=1}^{\infty} B_n \text{Sin}_n
\]

where the coefficients are given by,

\[
A_n = \langle \text{Cos}_n | \Psi' \rangle = \int_0^{\lambda} \text{Cos}_n(x) \, \psi(x) \, dx, \quad n = 0, 1, 2, \ldots
\]

\[
B_n = \langle \text{Sin}_n | \Psi' \rangle = \int_0^{\lambda} \text{Sin}_n(x) \, \psi(x) \, dx, \quad n = 1, 2, \ldots
\]
Fig. 5.2 Periodic function $\Psi$ and its corresponding Fourier spectrum fingerprint.

Example

Fourier approach to reconstruct a function.

https://www.google.com/imgres?imgurl=https://cdn.britannica.com/700x450/77/61777-004-EB9F8008.jpg&imgrefurl=https://www.britannica.com/science/Fourier-analysis&h=336&w=405&tbnid=NeK_PrElMD_gM:&q=fourier+decomposition&tbnh=124&tbnw=150&usg=AI4_-kTUhxMn1_ww00uN6cMc0zyhvn4CcCq&ved=1ahUKEwiFw4Tu3O3dAhXkz4MKHU0IABgQ_B0wHoECAYQEs..i&docid=kZqBYHoxSaKOA&itg=1&sa=X&ved=2ahUKEwiFw4Tu3O3dAhXkz4MKHU0IABgQ_B0wHoECAYQEs..i&w=405
Spatial domain

Frequency domain

https://www.reed.edu/physics/courses/Physics331.f08/pdf/Fourier.pdf
Notice

- In expression (13) above the explicit dependence of the functions on the variable $x$ can be omitted. That is, we can work simply with the functions $\cos_n$ instead of working with the numbers $\cos_n(x)$, whenever convenient.

- In the notation for the scalar product we use $\langle \cos_n \mid \Psi \rangle$ and not $\langle \cos_n(x) \mid \Psi(x) \rangle$. This is to emphasize that the scalar product is between functions and not between numbers.

- Using explicitly the expression for $\cos_o = \sqrt{\frac{1}{\lambda}}$ and, according to (14),

$$A_0 = \langle \cos_o \mid \Psi \rangle = \int_0^\lambda \cos_o(x) \psi(x) dx = \int_0^\lambda \sqrt{\frac{1}{\lambda}} \psi(x) dx$$

we realize that the first term in the Fourier series expansion gives,

$$A_0 \cos_o = \left( \int_0^\lambda \sqrt{\frac{1}{\lambda}} \psi(x') dx' \right) \left( \sqrt{\frac{1}{\lambda}} \right) = \frac{1}{\lambda} \int_0^\lambda \psi(x') dx' ,$$

which is nothing but the average value of the function $\Psi$ (average taken over one period). That is,

$$\Psi(x) = \frac{1}{\lambda} \int_0^\lambda \psi(x') dx' + \sum_{n=1}^\infty A_n \cos_n(x) + \sum_{n=1}^\infty B_n \sin_n(x) \quad (15)$$

**SUMMARY**

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

If we want to obtain $v_2$
\( \hat{e}_2 \cdot \mathbf{v} \quad \text{gives} \quad v_2 \)

In general
\( \hat{e}_j \cdot \mathbf{v} = v_j \); for \( j=1, 2,3 \)

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

- For a function \( \Psi \) of period \( \lambda \),
\[
\Psi(x) = A_0 \cos(x) + \sum_{n=1}^{\infty} A_n \cos(nx) + \sum_{n=1}^{\infty} B_n \sin(nx)
\]

or simply
\[
\Psi = A_0 \cos(x) + \sum_{n=1}^{\infty} A_n \cos(nx) + \sum_{n=1}^{\infty} B_n \sin(nx)
\]

If we want to obtain \( A_n \),
\[
\cos_n \cdot \Psi \quad \text{gives} \quad A_n
\]

\((\cos_n, \Psi)\)
\[ \langle \cos_n | \psi \rangle \]

\[ \lambda \int_0^\lambda \cos_n(x) \psi(x) \, dx \]

Just different notations for the same quantity

- \( \cos_0(x) \equiv \frac{1}{\sqrt{\lambda}} \),
- \( \cos_1(x) \equiv \sqrt{2} \cos(\frac{2\pi}{\lambda} x) \) \( k_1 = 1 \frac{2\pi}{\lambda} \)
- \( \cos_2(x) \equiv \sqrt{2} \cos(\frac{2\pi}{\lambda} x) \) \( k_2 = 2 \frac{2\pi}{\lambda} \)
- \( \cos_3(x) \equiv \sqrt{2} \cos(\frac{2\pi}{\lambda} x) \) \( k_3 = 3 \frac{2\pi}{\lambda} \)

Spatial frequency \( k \) of the corresponding harmonic function
5.1.C.b Spectral decomposition of *Non-periodic* Functions: The Fourier Integral

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

For an arbitrary function $\Psi$ of period $\lambda$, we have the Fourier series expansion,

$$\Psi(x) = A_0 \cos(x) + \sum_{n=1}^{\infty} A_n \cos(nx) + \sum_{n=1}^{\infty} B_n \sin(nx) \quad (15)$$

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

$$\Psi(x) = \frac{1}{\lambda} \int_{0}^{\lambda} \psi(x) dx + \sum_{n=1}^{\infty} A_n \sqrt{\frac{2}{\lambda}} \cos\left(\frac{2\pi}{\lambda/n} x\right) + \sum_{n=1}^{\infty} B_n \sqrt{\frac{2}{\lambda}} \sin\left(\frac{2\pi}{\lambda/n} x\right)$$

Since $\Psi$ and all the harmonic functions have period $\lambda$, we can change the interval of interest $(0, \lambda)$ to $(-\lambda/2, \lambda/2)$ instead, and thus re-write,
\[ \Psi(x) = \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} \psi(x') dx' + \sum_{n=1}^{\infty} A_n \left[ \sqrt{\frac{2}{\lambda}} \cos\left(\frac{n\pi}{\lambda} x\right) \right] + \sum_{n=1}^{\infty} B_n \left[ \sqrt{\frac{2}{\lambda}} \sin\left(\frac{n\pi}{\lambda} x\right) \right] \] \\

(15)'

where \( A_n = \langle \cos_n | \Psi \rangle = \int_{-\lambda/2}^{\lambda/2} \left[ \sqrt{\frac{2}{\lambda}} \cos\left(\frac{n\pi}{\lambda} x'\right) \right] \psi(x') dx' \), \( n=1,2, \ldots \)

\[ B_n = \langle \sin_n | \Psi \rangle = \int_{-\lambda/2}^{\lambda/2} \left[ \sqrt{\frac{2}{\lambda}} \sin\left(\frac{n\pi}{\lambda} x'\right) \right] \psi(x') dx' \), \( n=1,2, \ldots \)

Let's define

\[ k_o \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad k_n = nk_o \] 

(16)

Notice, when \( \lambda \to \infty \), the quantity \( k_o \equiv \frac{2\pi}{\lambda} \) becomes infinitesimally small.

Using (16), expression (15)' adopts the form,

\[ \Psi(x) = \frac{1}{\lambda} \int_{-\lambda/2}^{\lambda/2} \psi(x') dx' + \sum_{n=1}^{\infty} A_n \left[ \sqrt{\frac{2}{\lambda}} \cos(nk_o x) \right] + \sum_{n=1}^{\infty} B_n \left[ \sqrt{\frac{2}{\lambda}} \sin(nk_o x) \right] \] 

(15)'
where  
\[ A_n = \langle \cos_n \mid \psi' \rangle = \int_{-\lambda/2}^{\lambda/2} \left[ \sqrt{\frac{2}{\lambda}} \cos(nk_0x') \right] \psi(x') \, dx ; \quad n=1,2, \ldots \]

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

**Moving from the (discrete) variable \( n \) to the (continuum) \( k \) variable**

When \( \lambda \to \infty \), the value \( k_0 \equiv \frac{2\pi}{\lambda} \to 0 \). We justify below that

the “summation over \( n \)” in (15)'

**can become an**

**an “integral of the variable \( k = nk_0 \)”**.

**Strategy:**

- Instead of increasing \( k \) in units of \( k_0 \) (that is, increasing \( k \) by \( 1k_0 \) each time: \( k, k + k_0, k + 2k_0, k + 3k_0, \ldots \))
  we rather increase \( k \) in chunks of magnitude \( \Delta k \) (to thus speed up the calculation of the sum in expression (15)'). A large enough \( \Delta k \) will contain many discrete values of \( k \), still all the corresponding \( A_k \) and \( B_k \) will be approximately the same respectively.

- Let’s express the above strategy more quantitatively. In a range \( \Delta k \) there will be an integer number \( (\Delta k) / k_0 \) of terms that in the summation above will have a similar coefficient \( A_k \).

It is also convenient to use the index \( k \) instead of \( n \): \( A_n \) becomes \( A_k \).
Fig. 5.3 Transition of the Fourier component from discrete variable $n$ to a continuum variable $k$.

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

$$
\Psi(x) \underset{\lambda \rightarrow \infty}{\longrightarrow} \int_{0}^{\infty} \frac{\Delta k}{k_o} A_k \left[ \sqrt{\frac{2}{\lambda}} \cos(kx) \right] + \int_{0}^{\infty} \frac{\Delta k}{k_o} B_k \left[ \sqrt{\frac{2}{\lambda}} \sin(kx) \right]
$$

(17)

Or equivalent,

$$
\Psi' \underset{\lambda \rightarrow \infty}{\longrightarrow} \int_{0}^{\infty} \frac{\Delta k}{k_o} A_k \left[ \sqrt{\frac{2}{\lambda}} \cos_k \right] + \int_{0}^{\infty} \frac{\Delta k}{k_o} B_k \left[ \sqrt{\frac{2}{\lambda}} \sin_k \right]
$$

Summation (i.e. integration) is over the $k$ variable

where

$$
A_n \underset{\lambda \rightarrow \infty}{\longrightarrow} A_k = \int_{-\lambda/2}^{\lambda/2} \left[ \sqrt{\frac{2}{\lambda}} \cos(kx') \right] \psi(x') dx'
$$

$$
B_n \underset{\lambda \rightarrow \infty}{\longrightarrow} B_k = \int_{-\lambda/2}^{\lambda/2} \left[ \sqrt{\frac{2}{\lambda}} \sin(kx') \right] \psi(x') dx'
$$

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

$$
\Psi(x) \underset{\lambda \rightarrow \infty}{\longrightarrow} \int_{0}^{\infty} \frac{\Delta k}{k_o} \left[ \sqrt{\frac{2}{\lambda}} \int_{-\lambda/2}^{\lambda/2} \cos(kx') \psi(x') dx' \right] \left[ \sqrt{\frac{2}{\lambda}} \cos(kx) \right] +
$$

$A_k$

$$
+ \int_{0}^{\infty} \frac{\Delta k}{k_o} \left[ \sqrt{\frac{2}{\lambda}} \int_{-\lambda/2}^{\lambda/2} \sin(kx') \psi(x') dx' \right] \left[ \sqrt{\frac{2}{\lambda}} \sin(kx) \right]
$$

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

\[
\Psi(x) \xrightarrow{\lambda \to \infty} \int_{0}^{\infty} \Delta k \left[ \frac{1}{\pi} \int_{-\lambda/2}^{\lambda/2} \cos(kx') \psi(x') dx' \right] \cos(kx) + \\
+ \int_{0}^{\infty} \Delta k \left[ \frac{1}{\pi} \int_{-\lambda/2}^{\lambda/2} \sin(kx') \psi(x') dx' \right] \sin(kx)
\]

\[
\Psi(x) = \int_{0}^{\infty} dk \left[ \frac{1}{\pi} \int_{-\infty}^{\infty} \cos(kx') \psi(x') dx' \right] \cos(kx) + \\
+ \int_{0}^{\infty} dk \left[ \frac{1}{\pi} \int_{-\infty}^{\infty} \sin(kx') \psi(x') dx' \right] \sin(kx)
\]  \hspace{1cm} (18)

Or, equivalently

\[
\Psi(x) = \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} dk \left[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \cos(kx') \psi(x') dx' \right] \cos(kx) + \\
\underbrace{A(k)}_{\frac{1}{\sqrt{\pi}} \int_{0}^{\infty} dk \left[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \sin(kx') \psi(x') dx' \right] \sin(kx)}
\]

\[
+ \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} dk \left[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \sin(kx') \psi(x') dx' \right] \sin(kx)
\]  \hspace{1cm} (B(k))

In summary, using a continuum BASIS-SET of harmonic functions
\{ \cos_k, \sin_k ; \ 0 < k < \infty \} \tag{19}

where
\begin{align*}
\cos_k(x) &\equiv \cos(\kappa x) \quad \text{and} \quad \sin_k(x) \equiv \sin(\kappa x)
\end{align*}

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

\[
\varphi(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} A(k) \cos_k(x) \, dk + \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} B(k) \sin_k(x) \, dk
\tag{20}
\]

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

\[
A(k) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \varphi(x') \cos(kx') \, dx', \quad \text{and}
\]

\[
B(k) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \varphi(x') \sin(kx') \, dx'
\]
SUMMARY

\[ \Psi(x) = \frac{1}{\sqrt{\pi}} \int_{0}^{z} A(k) \cos_k(x) \, dk + \frac{1}{\sqrt{\pi}} \int_{0}^{z} B(k) \sin_k(x) \, dk \]

If we want to obtain \( A(k) \),

\[ \left( \frac{1}{\sqrt{\pi}} \cos_k, \Psi \right) \]

\[ \langle \frac{1}{\sqrt{\pi}} \cos_k | \Psi \rangle \]

\[ \frac{1}{\sqrt{\pi}} \int_{-z}^{z} \cos(kx') \psi(x') \, dx' , \]

**Exercise.** If expression (20) is correct, then

\[ \frac{1}{\pi} \int_{-z}^{z} \cos(kx) \cos(k'x) \, dx , = \delta(k-k') \]
where δ is the Delta Dirac

Answer:

Multiplying expression (20) by \( \frac{1}{\sqrt{\pi}} \cos(k'x) \) on both sides of the equality, and then integrating from \( x = -\infty \) to \( x = \infty \), we obtain,

In expression (18) above we have

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

which can also be expressed as,

\[ \Psi(x) = \int_0^\infty dk \frac{1}{\pi} \left[ \{ \cos(kx') \cos(kx) \} \psi(x') dx' + \right. \]
\[ + \int_0^\infty dk \frac{1}{\pi} \left[ \{ \sin(kx') \sin(kx) \} \psi(x') dx' \right. \]
\[ \Psi(x) = \int_0^\infty dk \frac{1}{\pi} \left[ \{ \cos(k(x'-x)) \} \psi(x') dx' \right. \]

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

\[ \Psi(x) = \int_0^\infty dk \left[ \frac{1}{\pi} \int_{-\infty}^{\infty} \cos(k(x'-x)) \psi(x') dx' \right] \quad (21) \]

\textbf{Even function in the variable} \( k \)

accordingly, we have the following identity,
\[
\int_{-\infty}^{\infty} dk \left[ \frac{1}{\pi} \int_{-\infty}^{x} \cos(k(x'-x)) \psi(x') dx' \right] = \\
= \int_{-\infty}^{0} dk \left[ \frac{1}{\pi} \int_{-\infty}^{x} \cos(k(x'-x)) \psi(x') dx' \right]
\]

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

Expression (21) can then be re-written as,

\[
\Psi(x) = \frac{1}{2} \int_{-\infty}^{x} dk \left[ \frac{1}{\pi} \int_{-\infty}^{x} \cos(k(x'-x)) \psi(x') dx' \right]
\]

(23)

On the other hand, notice the following identity,

\[
0 = -i \frac{1}{2} \int_{-\infty}^{x} dk \left[ \frac{1}{\pi} \int_{-\infty}^{x} \sin(k(x'-x)) \psi(x') dx' \right]
\]

(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

\[
\Psi(x) = \frac{1}{2\pi} \int_{-\infty}^{x} dk \int_{-\infty}^{x} \left[ \begin{array}{c} \cos(k(x'-x)) - i \sin(k(x'-x)) \end{array} \right] \psi(x') dx' \\
= e^{-ik(x'-x)}
\]

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

(25)

Rearranging the terms,

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

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

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

In summary, using the infinite and continuum basis-set of complex functions,

\[\text{BASIS-SET } \{ e_k, \ -\infty < k < \infty \} \]

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

an arbitrary function \( \Psi' \) can be expressed as a linear combination of such basis-set functions,

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

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

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

which is typically referred to as the Fourier transform of the function \( \Psi' \).

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

In essence, the Fourier formalism associates to a given function \( f \) its Fourier transform \( F \).
An important characteristic in the Fourier formalism is that, it turns out,

\[ f \leftrightarrow F \]

(29)

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

Fig. 5.4 Reciprocity between a function and its spectral Fourier transform.

Due to its important implication in quantum mechanics, this property (29) will be described in greater detail in the Section 5.2 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, later on when we identify (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.
5.1.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 $\Phi$ and $\psi$ be two arbitrary complex functions. The scalar product between $\Phi$ and $\psi$ is defined as follows,

$$\langle \Phi | \psi \rangle \equiv \int_{-\infty}^{\infty} \Phi^*(x) \psi(x) \, dx$$  \hspace{1cm} \text{definition of scalar product.} \hspace{1cm} (30)$$

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

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

that is,

$$\langle \Phi | \psi \rangle^* = \langle \psi | \Phi \rangle$$  \hspace{1cm} (31)$$

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

Notice that the corresponding Fourier-transform coefficient

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx'} \Psi(x') \, dx' = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left( e^{ikx'} \right)^* \Psi(x') \, dx'$$

can also be expressed in a more compact form (using the notation for scalar product) as

$$= \frac{1}{\sqrt{2\pi}} \langle e_k | \Psi \rangle$$  \hspace{1cm} (32)$$

where $e_k(x) \equiv e^{ikx}$
Thus, if $\Psi(x) = \int_{-\infty}^{\infty} F(k) \frac{1}{\sqrt{2\pi}} e^{ikx} \, dk$

which means

$|\Psi\rangle = \int_{-\infty}^{\infty} F(k) \frac{1}{\sqrt{2\pi}} e^{ik} \, dk$

and we want to find a particular component $F(k')$, we simply multiply $\Psi$ on the left by $\langle \frac{1}{\sqrt{2\pi}} e^{ik'} |$ and obtain

$\langle \frac{1}{\sqrt{2\pi}} e^{ik'} | \Psi \rangle = F(k')$

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

$$\Psi \leftarrow \text{equally represented by} \rightarrow |\psi\rangle$$

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

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

Further, the “ket” $|\frac{1}{\sqrt{2\pi}} e^{k} \rangle$ 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 $\Psi$ is a linear combination of the base-functions $\{\varphi_n; \ n = 1, 2, \ldots\}$. Thus, we can use the notation,

$$\Psi = \sum_n A_n \varphi_n \quad \text{or} \quad |\Psi\rangle = \sum_n A_n |\varphi_n\rangle \quad (33)$$

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 \( |\varphi_n\rangle \);

\[
|\psi\rangle = \sum_n |\varphi_n\rangle A_n
\]  

(33)

- Another alternative notation of (33) 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

\[
\langle \varphi_n | \psi \rangle = A_n
\]  

(34)

Accordingly,

\[
|\psi\rangle = \sum_n |\varphi_n\rangle A_n = \sum_n |\varphi_n\rangle \langle \varphi_n | \psi \rangle
\]  

(35)

### 5.2 PHASE VELOCITY and GROUP VELOCITY

Let’s start with a simple example.

**Question:** In the XYZ space, identify all the points \((x, y, z)\) such that their vector position is perpendicular to the unit vector \((1, 0, 0)\).

**Answer:** All the points on the “plane YZ that passes through \(x=0\)” fulfills that requirement.

Notice we can express the answer in an alternative way: “all points \(\mathbf{r} = (x, y, z)\) such that \(\mathbf{r} \cdot (1, 0, 0) = 0\)” fulfills that requirement.

**Question:** How to express mathematically the set of points \((x, y, z)\) located in the plane YZ that passes through the point 3(1, 0, 0).

**Answer:** All points \(\mathbf{r} = (x, y, z)\) such that \(\mathbf{r} \cdot (1, 0, 0) = 3\) fulfills that requirement.

**Question:** Identify all points \(\mathbf{r} = (x, y, z)\) such that \(\mathbf{r} \cdot (1, 0, 0) = 7\).

**Question:** Identify all points \(\mathbf{r} = (x, y, z)\) such that \(\mathbf{r} \cdot (1, 0, 0) = 9\).

**Question:** Identify all points \(\mathbf{r} = (x, y, z)\) such that \(\mathbf{r} \cdot (1, 1, 0) = 4\).

**Question:** Identify all points \(\mathbf{r} = (x, y, z)\) such that \(\mathbf{r} \cdot (1, 1, 0) = 0\).
Question: Identify all points \( \mathbf{r} = (x,y,z) \) such that \( \mathbf{r} \cdot (1,1,0) = -4 \).

5.2.A Planes

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

Notice, \[ \mathbf{r} \cdot \mathbf{n} = \text{const} \]

locates the points \( \mathbf{r} \) that constitute a plane oriented perpendicular to \( \mathbf{n} \).

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

**Fig. 5.5.** Left: A plane perpendicular to the unit vector \( \mathbf{n} \). Right: Different planes are obtained when using different values for the constant value \( c \) in the expression \( \mathbf{r} \cdot \mathbf{n} = c(\text{const}) \).

5.2.B Traveling Plane Waves and Phase velocity

Consider the two-variable vectorial function \( E \) of the form
\[ \mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \ f( \mathbf{r} \cdot \mathbf{n} - vt ) \]

where \( f \) is an arbitrary one-variable function and \( \mathbf{E}_0 \) is a constant vector.

For example, \( f \) could be the \( \cos \) function; i.e.

\[ \mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \ \cos( \mathbf{r} \cdot \mathbf{n} - vt ) \]

Notice, the points over a plane oriented perpendicular to \( \mathbf{n} \) and traveling with velocity \( v \) define the locus of points where the phase of the wave \( \mathbf{E} \) remains constant. For this reason, the wave \( \mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0 \ \cos( \mathbf{r} \cdot \mathbf{n} - vt ) \) is called a plane wave.

\textbf{Fig. 5.6} 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 \( \mathbf{n} \).

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 \( \text{COS, EXP, ...} \) etc.

\[ f(x - vt) \]

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

**Traveling Harmonic Waves**

\[ \text{COS}(kx - \omega t) = \text{COS} \left[ k(x - \frac{\omega}{k} t) \right] \quad \text{and} \quad e^{i(kx - \omega t)} \]

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.

5.2.C \textbf{A Traveling Wave-package and its Group Velocity}

Consider the expression

\[ f(x) = \left( \frac{1}{\sqrt{2\pi}} \right) \int_{-\infty}^{\infty} F(k) \ e^{ikx} \, dk \]

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 this pulse at a later time will be represented by,

\[ \psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \ e^{i(kx - \omega t)} F(k) \quad \text{Pulse composed by a group of traveling harmonic waves} \quad (36) \]

Since, each component \( e^{i(kx - \omega t)} \) of the group travels with its own phase velocity,
would still be 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 A: 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.

\[
\psi(x,t) = \cos[kx - \omega t] + \cos[(k + \Delta k)x - (\omega + \Delta \omega)t]
\]

(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

\[
\cos(A + B) + \cos(A - B) = 2\cos(A)\cos(B),
\]

which can be expressed as

\[
\cos(A) + \cos(B) = 2\cos\left(\frac{A + B}{2}\right)\cos\left(\frac{A - B}{2}\right)
\]

Accordingly, (38) can be expressed as,

\[
\psi(x,t) = 2\cos\left[\left(\frac{\Delta k}{2}\right)x - \left(\frac{\Delta \omega}{2}\right)t\right]\cos\left[(k + \frac{\Delta k}{2})x - (\omega + \frac{\Delta \omega}{2})t\right]
\]

Since we are assuming that \( \Delta \omega \ll \omega \) and \( \Delta k \ll k \), we have

\[
\psi(x,t) = 2\cos\left[\left(\frac{\Delta k}{2}\right)x - \left(\frac{\Delta \omega}{2}\right)t\right]\cos\left[kx - \omega t\right]
\]

(38)

\[\text{Modulation envelope}\]

Notice, the modulation envelope travels with velocity equal to

\[
v_g = \frac{\Delta \omega}{\Delta k},
\]

(39)

which is known as the group velocity.

In summary,
\[ \psi(x,t) = 2 \cos\left[ \frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t \right] \cos[ kx - \omega t ] \]  

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 whose \( k \)'s and \( \omega \)'s are very similar in value.
  - Case: Waves components of similar phase velocity, and group-velocity similar to the phase velocities.

Let,
\[
C(z, t) = \cos [ k_1 z - \omega_1 t ] = \cos [ 2 z - 5 t ] \tag{41}
\]
\[
D(z, t) = \cos [ k_2 z - \omega_2 t ] = \cos [ 2.1 z - 5.25 t ]
\]
Fig. 5.7a 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.

$$C = \cos (k_1 z - \omega_1 t)$$

$$D = \cos [(k_1 + \Delta k) z - (\omega_1 + \Delta \omega) t]$$

At $t=0.1$

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. 5.7b The profile of i) the individual waves $C(z, t)$ and $D(z, t)$ and ii) the profile of the sum $C(z, t) + D(z, t)$, are plotted at $t=0.1$ over the $0<z<75$ range.

$$k_1 = 2, \quad \Delta k = 0.1$$

$$\omega_1 = 5, \quad \Delta \omega = 0.25$$

$$V = \frac{\omega_1}{k_1} = 2.5$$
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 total wave \( C(z, t) + D(z, t) \) (the individual waves \( C \) and \( D \) are given in expression (41) above) is plotted at 2 different times in order to visualize the net motion of the interference profiles (group velocity).
Fig. 5.9 Notice, the net displacement of the valley is ~10 units, which occurs during an incremental time of 4 - 0.1 = 3.9 units. This indicates that the envelope profile travels with a velocity equal to 10 / 3.9 ~ 2.5. This value coincides with the value of \( \Delta \omega / \Delta k = 0.25/01 \).

**In the example above:**

The **phase velocity** of the individual waves are

\[
\frac{5}{2} = 2.5 \quad \text{and} \quad \frac{5.25}{2.1} = 2.5
\]

The **group velocity** as observed in the graph above is: 10 / 3.9 = 2.5

The **group velocity** as calculated from \( \Delta \omega / \Delta k \) is 2.5

**EXAMPLE-2:** Visualization of the addition of two waves whose \( k' \)'s and \( \omega' \)'s are very similar in value.

**Case:** Waves components of similar phase velocity, but group-velocity different than the phase velocity.

Let,

\[
C(z, t) = \cos(k_1 z - \omega_1 t) = \cos(2 z - 5 t)
\]

\[
D(z, t) = \cos(k_2 z - \omega_2 t) = \cos(2.1 z - 5.1 t)
\]

**GROUP VELOCITY = 2.5**

\( k_1 = 2 \quad \Delta k = 0.1 \quad C = \cos(k_1 z - \omega_1 t) \)

\( \omega_1 = 5 \quad \Delta \omega = 0.25 \quad D = \cos((k_1 + \Delta k) z - (\omega_1 + \Delta \omega) t) \)

\( V_{\text{phase}} = \omega_1 / k_1 = 2.5 \quad V_{\text{group}} = \Delta \omega / \Delta k = 2.5 \)
In the example above:

The phase velocity \( \omega / k \) of the individual waves are \( 5/2 = 2.5 \) and \( 5.1/2.1 = 2.42 \) respectively.

The group velocity as observed in the graph above is: 1

The observed group velocity coincides with \( \Delta \omega / \Delta k \) is 1

Comparing Fig. 5.9 and Fig. 5.10 we get evidence that the wavepackets of the first group velocity advances faster than the second group, 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. Below we show the method of phasors to add up multiple waves, which will help us understand, in a more simple way, how to represent a single pulse.
First, let's try to understand qualitatively, from a phasors addition point of view, how a train of (multiple) pulses is formed.

\[ \theta = kx - \omega t \]

**Fig. 5.10** A phasor representation in the complex plane.

**Example:** Let's consider the wave \( \Psi(x,t) = \cos(kx - \omega t) \) and analyze it at a given fixed time (t= 0.1 for example)

- **Analysis using only real variable**
  
  First we plot the profile of the wave at t=0.1

  Notice, as \( x \) changes the phase \((kx - \omega \times 0.1)\) changes.

- **Analysis using complex variable, phasors**
CASE-1: Wavepacket composed of two waves

Let’s consider the addition of two harmonic waves

\[
\Psi(x,t) = \cos(k_A x - \omega t) + \cos(k_B x - \omega t) \quad \text{Real} \tag{43}
\]

where, without losing generality, we will assume \( k_A < k_B \). Also, let’s call

\[ k_B - k_A \equiv \Delta k. \]

To evaluate (43) we will work in the complex plane. Accordingly, to each wave we will associate a corresponding phasor,

\[
\tilde{\Psi}(x,t) = e^{i(k_A x - \omega t)} + e^{i(k_B x - \omega t)} \quad \text{Complex} \tag{44}
\]

On the right side, each phasor component has magnitude equal to 1. (But below we will draw them as if they had slightly different magnitude just for clarity)

The projection of the (complex) phasors along the horizontal axis will give the real-value \( \Psi(x,t) \) we are looking for in (43).

Notice in (44) that,

\[
\tilde{\Psi}(x,t) = [e^{i k_A x} + e^{i k_B x}] e^{-i \omega t}
\]

Hence, we can analyze first only the factor \([e^{i k_A x} + e^{i k_B x}]\). One can always add the factor \( e^{-i \omega t} \) later on.

\[
\tilde{\Psi}(x) = [e^{i k_A x} + e^{i k_B x}] \tag{45}
\]
Notice that at a given position \( x \), the phase-difference between the two wave components is equal to,

\[
\text{Phase difference} = k_B x - k_A x
\]

(46)

\[
= (k_B - k_A) x
\]

The following happens:

\textbf{a) Real analysis for } t=0 \text{ and different values of } x

According to (43), at \( x = 0 \) both waves have the same phase equal to zero. The waves then interfere constructively there. So \( x = 0 \) is the first point of constructive interference.

\textbf{Complex (phasor) analysis:} Similarly, since the phase of each of the two waves in (45) is the same at \( x = 0 \), the corresponding phases will be aligned to each other (see figure below). Thus the amplitude of the total phasor, associated to \( x = 0 \), is maximum.

Graphically, at \( t = 0 \) and \( x = 0 \) we will have,
At $x = 0$ and $t > 0$ we will have:

Variation of the phases as time changes.

Now, let’s keep the time fixed at $t = 0$.

b) **Variation of the phases as the position $x$ changes**

As $x$ increases a bit, the interference is not as perfect (amplitude is less than 2) since the phase of the waves start to differentiate from each other; $(k_B - k_A)x \neq 0$. 
**Fig. 5.11** 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. Notice, once a value of \( x \) is chosen and left fixed, as the time advances all the phasors will rotate clockwise at angular velocity \( \omega \).

\[
\begin{align*}
k_B x - k_A x
\end{align*}
\]

c) As \( x \) increases, it will reach a particular value \( x = x_1 \) that makes the phase difference between the waves equal to \( 2\pi \). 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. 5.12** Left: In general, at arbitrary value of \( x \), the phasors do not coincide. Right: At a particular specific value \( x = x_1 \), 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 \( x = x_1 \).

\[
\Psi(x) = \cos(k_1x) + \cos(k_2x)
\]

**Fig. 5.13** Wavepacket composed of two harmonic waves. Here \( x_1 = 2\pi/(k_2 - k_1) \).

**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 \((x_1, x_2, x_3, \ldots)\) will be found to produce additional maxima.
**Case II: A wavepacket composed of several harmonic waves**

When adding several harmonic waves $\Psi(x) = \sum_{i=1}^{M} A_i \cos(k_i x)$, 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 $x=0$.
- The next position $x=x_1$ where maximum interference occurs will be one where the following condition is fulfilled

$$ (k_i - k_j) x_1 = (\text{integer}) ij \ 2\pi \quad (47) $$

for all the $ij$ combinations, with $i$ and $j = 1, 2, 3, \ldots, M$.

When condition (47) is fulfilled, all the corresponding phasors coincide, thus giving a maximum of amplitude for the wavepacket at $x=x_1$.

If we had wavepackets of the same frequency range $\Delta k$, expression (47) implies that a greater value of $x_1$ may be needed any time extra number of harmonic waves are included in the packet. That is, the “bumps” in Fig. 5.13 will be more separated, as suggested in Fig. 5.14.

- Third, additional regions of maximum interference will occur at multiple integers of $x_1$.

**Fig. 5.14** Wavepacket composed of a large number of harmonic waves. The train of pulses in the $x$-space are more separated from each other (when compared with the case of Fig. 5.13 above) because the individual $k$ vectors are closer between each other. Here $x_1 = 2\pi / \delta$

Notice also that, for an arbitrary position $x$ where the is not maximum interference, the greater the number of harmonic components in the wavepacket $\Psi$ (with wavevectors $k_i$ within the same range $\Delta k$ shown in the figure above), the stronger tendency of the $\Psi(x)$ value to have an average equal to zero.
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 $\Delta k$), the more separated from each other will be the regions of constructive interference. This is shown in Fig. 5.14.

**Case: Wavepacket composed of an infinite number of harmonic waves**

Adding more and more wavevectors $k$ (still all of them within the same range $\Delta k$) 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.

![Wavepacket composed of wavevectors $k$ within a continuum range $\Delta k$ produces a single pulse.](image)

**Fig. 5.15** Wavepacket composed of wavevectors $k$ within a continuum range $\Delta k$ produces a single pulse.

What about the variation of the pulse-size as $\Delta$ increases?

Fig. 5.15 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 $x$ had a very small value; 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 $\Delta k$, the corresponding range $\Delta x$ 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:

A wavepacket \( \Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} F(k) e^{ikx} \, dk \) has the following property,

\[
\Delta x \sim \frac{1}{\Delta k} \tag{48}
\]

In the expression for the wavepacket, \( x \) is interpreted as the position coordinate and \( k \) as spatial-frequency. Mathematically, we can also express a temporal pulse as

\[
\phi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} A(\omega) e^{i\omega t} \, d\omega ,
\]

so also we expect the following relationship,

\[
\Delta t \sim \frac{1}{\Delta \omega} \tag{48}'
\]
Expressions (48) and (48)' are general properties of the Fourier analysis of waves. In principle, they have 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 (λ and ν, to be more specific) are identified (via the de Broglie wave-particle duality hypothesis, to be expressed below) with the particle’s physical variables (p and E). Once this is done, then p and E) become subjected to the relationship indicated in (48) and (48)'.

The fact that physical variables are subjected to the relationships like in (48) and (48)' constitute one of the cornerstones of Quantum Mechanics. We will explore this concept in the following section.

5.3 DESCRIBING the MOTION of a FREE PARTICLE in the context of the WAVE-PARTICLE DUALITY

According to Louis de Broglie, a particle of linear momentum \( p \) and total energy \( E \) is associated with a wavelength \( \lambda \) and a frequency \( \nu \) given by,

\[
\lambda = \frac{h}{p} \quad \text{where} \quad \lambda \quad \text{is the wavelength of the wave associated with the particle’s motion; and}
\]

\[
\nu = \frac{E}{h} \quad \text{the total energy} \quad E \quad \text{is related to the frequency} \quad \nu \quad \text{of the wave associated with its motion.}
\]

where \( h \) is the Planck’s constant; \( h = 6.6 \times 10^{-34} \text{Js} \).

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 complicated 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) let’s 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 motion of a free particle.
5.3.A Proposition-1: Using a wavefunction with a definite linear momentum

- Taking into account the associated de Broglie’s wavelength $\lambda$ and frequency $\nu$, let’s construct (by making an arbitrary guess) a wavefunction of the form,$^2$

$$\psi(x,t) = ACos \left[ \frac{2\pi}{\lambda} x - 2\pi \nu t \right]$$

$$\mathcal{E}(x,t) = \mathcal{E}_o Cos \left[ \frac{2\pi}{\lambda} x - \nu t \right]$$

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 $|\mathcal{E}(x,t)|^2$.

- This (guessed) wavefunction (49) is proposed following an analogy to the description of electromagnetic waves,

$$\mathcal{E}(x,t) = \mathcal{E}_o Cos \left[ \frac{2\pi}{\lambda} x - \nu t \right]$$

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 $v_{\text{classical}}$, would we get the same value (somehow) from the wavefunction $\psi(x,t)$ given in (49)?

First, notice for example that the wavefunction (49) has a phase velocity given by,

$$v_{\text{wavefunction}} = E / p \quad \text{(phase velocity)}$$

On the other hand, let’s calculate the value of $E/p$ for a non-relativistic classical particle,

$$E = \frac{1}{2} m \left(v_{\text{classical}}\right)^2, \quad \text{and} \quad p = m \cdot v_{\text{classical}},$$

which gives,

$$E / p = \frac{1}{2} v_{\text{classical}}$$

From (51) and (52), one obtains,
\[ V_{\text{wavefunction}} = \frac{1}{2} V_{\text{classical}} \] (53)

We realize here a \textbf{disagreement} between the velocity of the particle \( V_{\text{classical}} \) and the phase velocity of the wave-particle \( V_{\text{wavefunction}} \) that is supposed to represent the particle.

This apparent shortcoming may be attributed to the fact that the proposed wavefunction (49) has a definite momentum \( p \) (and thus an infinite spatial extension). A better selection of a wavefunction has to be made then in order to describe a particle more localized in space. That is explored in the next section.

\subsection*{5.3.B Proposition-2: Using a wave-packet as a wave-function}

Let’s assume our classical particle of mass \( m \) is moving with velocity

\[ V_{\text{classical}} = V_o \quad \text{\textit{classical velocity}} \] (54)

(or approximately equal to \( V_o \)).

Let’s build a wavefunction in terms of the value \( V_o \).

To represent this particle, let’s build a Fourier wave-packet such that,

\( i \) Its dominant harmonic component is one with

- wavelength \( \lambda_o = h / mv_o \), or
- wavenumber \( k_o = 2\pi / \lambda_o = (2\pi / h)mv_o \) \quad (55)

or, equivalently, in terms of the variable \( p \),

\( ii \) Its dominant harmonic component has

- momentum \( p = p_o = mv_o \) \quad (56)

That is, we would choose an amplitude \( A(p) \) that peaks when \( p \) is equal to the classical value of the particle’s momentum.

In the meantime, the width \( \Delta x \) and \( \Delta p \) of the wave packet are, otherwise, arbitrary.
Accordingly, we start building a wave-packet of the form:

\[ \psi(x,t) \sim \int \mathcal{A} \cos \left( \frac{2\pi}{\lambda} x - 2\pi vt \right) d\lambda \]

In terms of the momentum variable \( p = h/\lambda \) and energy \( \gamma = E/h \)

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

where \( E = E(p) = p^2 / 2m \) for we are considering a free no relativistic particle case.

Using the variables

\[ k \equiv \frac{2\pi}{h} p \quad \text{and} \quad \omega \equiv \frac{2\pi}{h} E, \quad (57) \]

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

\[ \psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\Delta k} A(k) e^{i[(kx-\omega t)]} dk \quad (58) \]

Whose dominant harmonic component is \( k = k_o \) given in (55),

\[ k_o = \frac{2\pi}{\lambda_o} = \left( \frac{2\pi}{h} \right) mv_o. \]

The group velocity of this wave-packet is given by, \( v_{\text{wavefunction's group-velocity}} = \frac{d\omega}{dk} \). Therefore we need to find an expression for \( \omega \) as a function of \( k \).

**CASE:** For a non-relativistic free particle \( E = \frac{p^2}{2m} \).

Using (57), we obtain,
\[ \omega(k) = \frac{2\pi}{\hbar} E = \frac{2\pi}{\hbar} \frac{p^2}{2m} = \frac{h}{2\pi} \frac{k^2}{2m} \]

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

\[ v_{\text{wave function’s group-velocity}} = \left. \frac{d\omega}{dk} \right|_{k_0} = \frac{h}{2\pi m} k_0 \]  

(59)

Using (57),

\[ v_{\text{wave function’s group-velocity}} = \left. \frac{d\omega}{dk} \right|_{k_0} = \frac{p_0}{m} = v_o \]  

(60)

Comparing this expression with expression (54), we realize that the wavepacket (58) represents better the non-relativistic particle, since the classical velocity is recovered through the group-velocity of the wavefunction.

The multiple-frequency wave-packet (58), instead of the single frequency expression (49,) represents better the particle since, at least for the moment, its group-velocity coincides with classical velocity of the particle.

Consequences: THE PARAGRAPH BELOW IS VERY IMPORTANT!

Notice, if a wave-packet (composed of harmonic waves with momentum-values \( p \) within a given range \( \Delta p \)) is going to represent a particle, then, according to the Fourier analysis there will be a corresponding extension \( \Delta x \) (wavepacket spatial width), which could be interpreted as the particle’s position. That is, there will not be a definite ‘exact’ position to be associated with the particle, but rather a range of possible values (within \( \Delta x \)). In short, there will be 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, allowing 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 (48) and (48)’ above), which has profound consequences in our view of the mechanics governing Nature.

Indeed, from (53) \( \Delta k \equiv \frac{2\pi}{\hbar} \Delta p \); thus \( \Delta x \sim \frac{1}{\Delta k} \) implies \( \Delta x \sim \frac{1}{2\pi \Delta p} = \frac{\hbar}{\Delta p} \), where we have defined \( \hbar \equiv \hbar / 2\pi \).
\[ \Delta x \sim \frac{\hbar}{\Delta p} \] implies that the better we know the momentum of the particle (that is, the narrower the range \( \Delta p \) in the wavepacket), the larger uncertainty \( \Delta x \) to locate the particle.

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 \( \Delta x \) and \( \Delta p \) 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 constrains that (55) implies: we can not improve the accuracy in knowing \( \Delta x \) without scarifying the accuracy of \( \Delta p \), and vice versa. In the next chapter we will further familiarize with this new quantum behavior.

**Summary:**

In this chapter we have tried to figure out a wavefunction that describes the motion of a free particle.

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,

\[ \lambda = \frac{\hbar}{p} \quad \text{where} \quad \lambda \quad \text{is the wavelength of the wave associated with} \quad \text{the particle’s motion; and} \]

\[ \nu = \frac{E}{\hbar} \quad \text{the total energy} \quad E \quad \text{is related to the frequency} \quad \nu \quad \text{of the wave associated with its motion.} \]

where \( \hbar \) is the Planck’s constant; \( \hbar = 6.6 \times 10^{-34} \) Js.

We found that associating the particle with a wave \( \mathcal{E}(x,t) = \mathcal{E}_0 \cos \left( \frac{2\pi}{\lambda} x - \nu t \right) \) of single spatial frequency \( k = 2\pi/\lambda \) and single temporal frequency \( \nu \), leads to an unacceptable result (the classical particle and the wavepacket traveling at different speed). Here \( \nu \) and \( k \) (or \( p \) and \( E \)) are related through \( E = p^2/2m \) in the case of a non-relativistic free particle.

As an alternative, a wavepacket \( \psi(x,t) \sim \int_{\Delta p} A(p) \cos \left( \frac{2\pi}{\hbar} (px - Et) \right) dp \) of width \( \Delta p \) was then postulated to represent a particle. The wavepacket would have a main component at \( p = p_{\text{classical}} \) and a width \( \Delta p \). When calculating the group velocity of this wavepacket at \( p = p_{\text{classical}} \) it turns out to be equal to the classical velocity. That is, the classical particle and the wavepacket travel at the same speed).
APPENDIX

Variations in the wavepacket for different spectral contents
Credit graphic results: Joseph Scotto
### Table 2: 1A) functions and corresponding k values. The wavepackets were constructed using Eq. (1) and the information in Table 1.

<table>
<thead>
<tr>
<th>Function</th>
<th>k Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Psi_I$</td>
<td>7, 8, 9</td>
</tr>
<tr>
<td>$\Psi_{II}$</td>
<td>6, 7, 8, 9, 10</td>
</tr>
<tr>
<td>$\Psi_{III}$</td>
<td>5, 6, 7, 8, 9, 10, 11</td>
</tr>
<tr>
<td>$\Psi_{IV}$</td>
<td>4, 5, 6, 7, 8, 9, 10, 11, 12</td>
</tr>
<tr>
<td>$\Psi_V$</td>
<td>3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13</td>
</tr>
</tbody>
</table>

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**1A: Spectral decomposition of an arbitrary function $\Psi$: Increasing the total spectral width (but keeping constant the spectral distance $\Delta k$ between the spectral components.)**

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Conclusion

Case: Total spectral width increases.

Notice the spatial large peaks do not get narrower (actually the spatial-width remains constant.) This occurs because the distance $\Delta k$ between spectral components remains constant.

Since the distance $\Delta k$ between spectral components is constant, the distance between the large peaks $(2\pi/\Delta k)$ remains constant.

Adding more $k$'s:

i) decreases the 'noise" in between the large peaks;

but

ii) do not change the position of the large peaks.
Case: Constant total spectral width.

Since the distance $\Delta k$ between spectral components decreases, the distance between the large peaks ($2\pi/\Delta k$) increases.

Adding more k's within the same total spectral range do not decreases the 'noise" in between the large peaks.

The width of the central spatial peak appears to remain the same.
Table 4: 1C) functions and corresponding $k$ values. The wavepackets were constructed using Eq. (1) and the information in Table 1.

<table>
<thead>
<tr>
<th>Function</th>
<th>$k$ Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Psi_i$</td>
<td>3.00, 3.50, 4.00, 4.50, 5.00, 5.50, 6.00, 6.50, 7.00, 7.50, 8.00, 8.50, 9.00</td>
</tr>
<tr>
<td>$\Psi_{ii}$</td>
<td>4.00, 4.33, 4.67, 5.00, 5.33, 5.67, 6.00, 6.33, 6.67, 7.00, 7.33, 7.67, 8.00</td>
</tr>
<tr>
<td>$\Psi_{iii}$</td>
<td>5.00, 5.17, 5.33, 5.50, 5.67, 5.83, 6.00, 6.17, 6.33, 6.50, 6.67, 6.83, 7.00</td>
</tr>
</tbody>
</table>

Same number of spectral components

Larger spectral bandwidth.

Smaller spectral bandwidth.

More localized spatial central peak.

Less localized spatial central peak.
OVERALL CONCLUSION

The granularity $D_k$ (distance between spectral components) determines the distance between large peaks.

The total spectral width determines the noise between peaks and the width of the spatial central peak.

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1 A more general concept of the wave-particle duality is the PRINCIPE of COMPLEMENTARY. See, for example, the following excellent reference: M. O. Scully, B. G. Englert, and H. Walther. “Quantum Optical Test of Complementary.” *Nature* **351**, 111 (1991).

2 Here we follow closely Quantum Physics, Eisberg and Resnick, Section 3.2