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The Motion of Wave Packets: Fourier Analysis

Because we will need to work with wave packets of finite extent, it will be very useful to first give a brief review of Fourier analysis.

A Fourier Series

We shall start by studying periodic functions of infinite extent in space. First consider periodic functions $f(x)$ with a periodicity interval 2π, such that $f(x+2\pi) = f(x)$. For real functions $f(x)$, we usually use Fourier expansions in cosine and sine functions. For the complex functions of quantum theory, it will be advantageous to use a Fourier expansion in exponential functions.

1. Fourier Expansion:

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{inx}, \tag{1}$$

where we will exploit the orthogonality of the exponential functions.

2. Orthogonality:

$$\int_{-\pi}^{\pi} dx' e^{i(n-m)x'} = 2\pi \delta_{nm}, \tag{2}$$

which is expressed in terms of the usual Kronecker delta. With this orthogonality relation, the expansion coefficients, a_n, can be determined via the Fourier inversion theorem. If we multiply $f(x)$ by the complex conjugate of a specific exponential, say, e^{-imx}, with some specific, fixed m, and integrate both sides of the resultant

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equation over the periodicity interval, say, from $-\pi$ to $+\pi$, the orthogonality property will pick out one specific a_m, with value given by the Fourier coefficients.

3. Fourier coefficients:

$$a_m = \frac{1}{2\pi} \int_{-\pi}^{\pi} dx' f(x') e^{-imx'}. \tag{3}$$

Substituting this coefficient back into the Fourier expansion, we get the

4. Fourier expression for $f(x)$:

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{1}{2\pi} \int_{-\pi}^{\pi} dx' f(x') e^{in(x-x')}. \tag{4}$$

It will be convenient to introduce orthonormal functions, $\phi_n(x)$,

$$\phi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx}. \tag{5}$$

The four basic Fourier equations can then be rewritten as

$$f(x) = \sum_{n=-\infty}^{\infty} b_n \phi_n(x), \tag{6}$$

$$\int_{-\pi}^{\pi} dx' \phi_n^*(x') \phi_m(x') = \delta_{nm}, \tag{7}$$

$$b_n = \int_{-\pi}^{\pi} dx' f(x') \phi_n^*(x'), \tag{8}$$

$$f(x) = \sum_{n=-\infty}^{\infty} \int_{-\pi}^{\pi} dx' f(x') \phi_n(x) \phi_n^*(x'). \tag{9}$$

Finally, it will be convenient to use a periodicity interval of length $(2l)$, where l has the dimension of a length, where now $f(x + 2l) = f(x)$ and the orthonormal functions can be expressed as

$$\frac{1}{\sqrt{2l}} e^{\frac{in\pi x}{l}}.$$

The four basic Fourier equations can then be rewritten as

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \frac{1}{\sqrt{2l}} e^{\frac{in\pi x}{l}}, \tag{10}$$

$$\frac{1}{2l} \int_{-l}^{+l} dx' e^{i(n-m)\frac{\pi x'}{l}} = \delta_{nm}, \tag{11}$$

$$c_n = \frac{1}{\sqrt{2l}} \int_{-l}^{+l} dx' f(x') e^{-i\frac{n\pi x'}{l}}, \tag{12}$$

$$f(x) = \frac{1}{2l} \sum_{n=-\infty}^{\infty} \int_{-l}^{+l} dx' f(x') e^{i\frac{n\pi}{l}(x-x')}. \tag{13}$$

It will now be useful to introduce the wavenumber, k_n

$$k_n = \frac{n\pi}{l} = \frac{2\pi}{\lambda_n}; \qquad \text{with} \quad \lambda_n = \frac{2l}{n}, \tag{14}$$

so $\phi_n(x) = \frac{1}{\sqrt{2l}} e^{ik_n x}$. This relation will be particularly useful in making the transition from the Fourier series to the Fourier integral for a wave packet of finite extent.

B Fourier Integrals

Now suppose the repeating function, with periodicity interval ($2l$), has the form of a wave packet of extent $\sim a$, with $a < l$, which repeats from $-\infty$ to $+\infty$, as shown in Fig. 2.1. Now, suppose we let $l \to \infty$, keeping the wave packet unchanged, with a fixed. Then, by taking the limit $l \to \infty$, provided $f(x) \to 0$ sufficiently rapidly as $x \to \pm\infty$, we can make the transition from a periodic function to a nonperiodic one, i.e., a transition from an infinite wave train to a wave packet of finite extent in space. As $l \to \infty$, the spectrum of possible k_n goes from a discrete spectrum to a continuous one, because

$$k_{n+1} - k_n = \frac{\pi}{l} \to 0 \qquad \text{as} \quad l \to \infty. \tag{15}$$

Because the number of spectral terms in a k-space interval dk is (see Fig. 2.2)

$$\frac{dk}{(\text{interval between successive } \mathrm{k_n})} = \frac{dk}{\pi/l},$$

the discrete sum over n in the Fourier series goes over to a continuous integral

$$\sum_{n=-\infty}^{\infty} \to \int_{-\infty}^{\infty} \frac{dk}{\pi/l}.$$

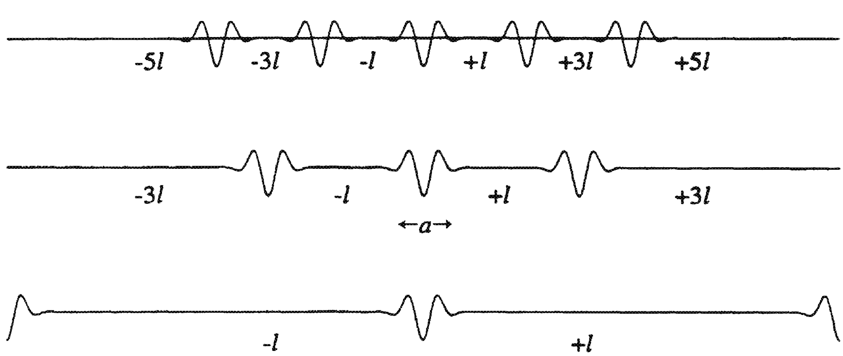

FIGURE 2.1. Periodic wave form, $l \to \infty$, a fixed.

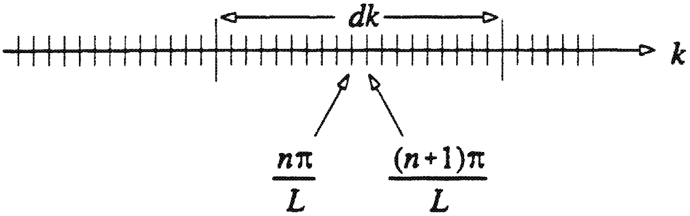

FIGURE 2.2. The spectrum of k values, $k_n = n\pi/L$. The number of spectral terms in the dk interval $= \left[dk/\frac{\pi}{L}\right]$.

Thus, the Fourier expression for $f(x)$ becomes

$$f(x) = \frac{1}{2l}\frac{l}{\pi}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' f(x') e^{ik(x-x')}. \tag{16}$$

We can then think of the Fourier development in terms of a Fourier amplitude function, $g(k)$, as

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk g(k) e^{ikx}, \tag{17}$$

with amplitude function $g(k)$, the so-called Fourier transform of $f(x)$, given by

$$g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx' f(x') e^{-ikx'}. \tag{18}$$

Note, however, the orthonormality integral becomes divergent when $k = k'$,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dx' e^{ix'(k-k')} = \delta(k - k'). \tag{19}$$

The Kronecker delta becomes a Dirac delta function.

C The Dirac Delta Function

If we rewrite the Fourier series in terms of a limit of a sum over a finite number of terms,

$$f(x) = \lim_{N\to\infty}\int_{-\pi}^{\pi} dx' f(x') \sum_{n=-N}^{+N} \phi_n(x)\phi_n^*(x'); \tag{20}$$

or, similarly, if we rewrite the Fourier integral as

$$f(x) = \lim_{k_0\to\infty}\int_{-\infty}^{\infty} dx' f(x') \frac{1}{2\pi}\int_{-k_0}^{k_0} dk e^{ik(x-x')}, \tag{21}$$

the function

$$K(x,x') = \sum_{n=-N}^{+N} \phi_n(x)\phi_n^*(x') \qquad \text{or} \qquad K(x,x') = \frac{1}{2\pi}\int_{-k_0}^{+k_0} dk e^{ik(x-x')} \tag{22}$$

becomes, in the limit of large N or large k_0, a function strongly peaked at $x = x'$ with oscillations of very small amplitude for $x \neq x'$. Keeping in mind that the real limiting processes should be those expressed by eqs. (20) and (21), physicists blithely interchange the infinite sum or the infinte k-integral with the x'-integral, through the definition of the Dirac delta "function"

$$\sum_{n=-\infty}^{\infty} \phi_n(x)\phi_n^*(x') = \delta(x-x')$$
$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik(x-x')} = \delta(x-x'), \tag{23}$$

where the Dirac delta "function" is not at all a function in the mathematician's sense. It is what mathematicians call a "distribution" (see, e.g., an appendix in Vol. I of the books by Messiah). The Dirac delta function "picks out" the value $x' = x$ for the function being integrated. It has meaning only through the integrals. By itself, it diverges at the value $x' = x$. The Dirac delta function is defined through the following properties:

$$\delta(x-x') = 0 \qquad \text{for} \qquad x' \neq x. \tag{24}$$

For $x' = x$, the Dirac delta function becomes ∞ in such a way that

$$\int_a^b dx'\delta(x-x') = 1, \qquad \text{if} \quad x' = x \text{ is in the interval } (a,b), \tag{25}$$

and

$$\int_{-\infty}^{\infty} dx' f(x')\delta(x-x') = f(x). \tag{26}$$

Our limiting process, given through eq. (21), e.g., would give

$$\delta(x-x') = \lim_{k_0\to\infty} \frac{1}{2\pi}\int_{-k_0}^{k_0} dk e^{ik(x-x')} = \lim_{k_0\to\infty} \frac{\sin k_0(x-x')}{\pi(x-x')}. \tag{27}$$

See Fig. 2.3 for a plot of this diffraction-like peaked function for finite k_0. This representation of the Dirac delta function is not, however, unique. Another example (of the infinite number of possibilities) would be

$$\delta(x-x') = \frac{1}{\pi}\lim_{\epsilon\to 0}\frac{\epsilon}{[(x-x')^2+\epsilon^2]}. \tag{28}$$

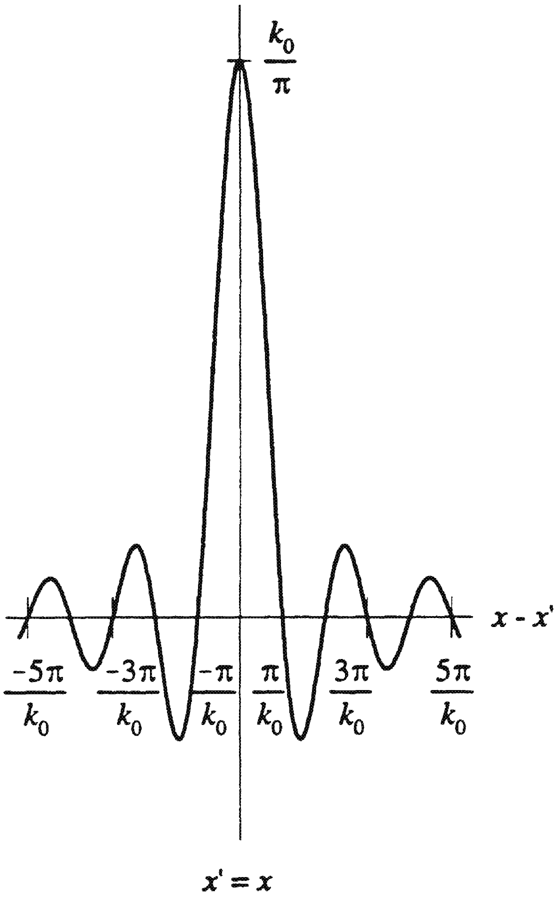

FIGURE 2.3. The function $\frac{\sin[k_0(x-x')]}{\pi(x-x')}$.

D Properties of the Dirac Delta Function

The Dirac delta function is an even function of its argument

$$\delta(-x) = \delta(x). \tag{29}$$

Other properties, such as

$$x\frac{d}{dx}\delta(x) = -\delta(x), \tag{30}$$

follow by integration by parts, because delta function relations have meaning only through their applications within integrals

$$\int_a^b dx x\delta'(x) = \Big[x\delta(x)\Big]_a^b - \int_a^b dx\delta(x) = -\int_a^b dx\delta(x). \tag{31}$$

If a is a real number,

$$\delta(ax) = \frac{1}{|a|}\delta(x). \tag{32}$$

Note the absolute value sign follows from

$$\int_{-\infty}^{\infty} dx\delta(ax) = \frac{1}{a}\int_{-\infty}^{\infty} d(ax)\delta(ax) = \pm\frac{1}{a}\int_{-\infty}^{\infty} dx'\delta(x'), \tag{33}$$

where the upper sign applies for $a > 0$ and the lower sign applies for $a < 0$, because the change of variable $ax = x'$ interchanges the limits in this latter case. If the variable in the delta function is itself a function of x,

$$\delta(\phi(x)) = \sum_n \frac{1}{|(\frac{d\phi}{dx})_{x_n}|}\delta(x - x_n), \tag{34}$$

where the x_n are the zeros of the function, $\phi(x)$, and the sum is a sum over all such zeros. As a very specific example,

$$\delta(x^2 - a^2) = \frac{1}{2|a|}\big[\delta(x - a) + \delta(x + a)\big]. \tag{35}$$

E Fourier Integrals in Three Dimensions

It is straightforward to generalize the Fourier series and Fourier integrals to functions in our three-dimensional (3-D) space, $f(x, y, z)$. For a 3-D wave packet,

$$f(x, y, z) = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty} dk_x\int_{-\infty}^{\infty} dk_y\int_{-\infty}^{\infty} dk_z\int_{-\infty}^{\infty} dx'\int_{-\infty}^{\infty} dy'$$
$$\times\int_{-\infty}^{\infty} dz' f(x', y', z')e^{i[k_x(x-x')+k_y(y-y')+k_z(z-z')]}. \tag{36}$$

It will be useful to introduce the following shorthand notation for this Fourier integral expression

$$f(\vec{r}) = \frac{1}{(2\pi)^3}\int d\vec{k}\int d\vec{r}\,' f(\vec{r}\,')e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}, \tag{37}$$

where

$$f(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d\vec{k}g(\vec{k})e^{i(\vec{k}\cdot\vec{r})}, \tag{38}$$

$$g(\vec{k}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d\vec{r}\,' f(\vec{r}\,')e^{-i(\vec{k}\cdot\vec{r}\,')}. \tag{39}$$

(Note, in particular, the symbol, $d\vec{r}$, when it follows an integral sign, is merely a shorthand notation for $d\vec{r} \equiv dxdydz$ and the single integral sign preceding $d\vec{r}$ is shorthand for a triple integral over all of 3-D space.)

F The Operation $\frac{1}{i}\frac{\partial}{\partial x}$

We note

$$\frac{1}{i}\frac{\partial}{\partial x}f(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d\vec{k}g(\vec{k})k_x e^{i(\vec{k}\cdot\vec{r})}. \tag{40}$$

Thus, we see, if $g(\vec{k})$ is the Fourier transform of $f(\vec{r})$, $\vec{k}g(\vec{k})$ is the Fourier transform of $\frac{1}{i}\vec{\nabla} f(\vec{r})$, similarly, $-(\vec{k}\cdot\vec{k})g(\vec{k})$ is the Fourier transform of $\nabla^2 f(x, y, z)$, and so on.

G Wave Packets

A plane scalar wave propagating in the direction of the $\vec{k}$ vector can be given by the scalar function

$$\psi(\vec{r}, t) = Ae^{i(\vec{k}\cdot\vec{r}-\omega t)}, \tag{41}$$

with constant amplitude, A, where the circular frequency, ω, is in general related to $\vec{k}$ through the dispersion law

$$\omega = f(\vec{k}), \qquad \text{or} \quad \omega = f(k), \quad \text{with} \quad k = |\vec{k}|, \tag{42}$$

where the latter is valid for an isotropic medium. Moreover, in a nondispersive medium, in vacuum, e.g., $\omega = ck$.

To go from this infinite wave train to a wave packet of finite extent in space, we need to form the wave packet from a superposition of amplitudes with different $\vec{k}$-values. For a 3-D wave packet,

$$\psi(\vec{r}, t) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d\vec{k}A(\vec{k})e^{i(\vec{k}\cdot\vec{r}-\omega t)}. \tag{43}$$

To simplify the discussion, assume the wave packet proceeds in one dimension only, say, the x-direction. Then,

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dkA(k)e^{i(kx-\omega t)}. \tag{44}$$

To use a very simple example, assume $A(k)$ is different from zero only in an interval, $k_0 - \frac{1}{2}\Delta k \leq k \leq k_0 + \frac{1}{2}\Delta k$, and moreover, assume $A(k)$ has the constant value, A, in this k-space interval. If the interval Δk is not too large, we can expand $\omega(k)$ about k_0, and retain only the dominant terms,

$$\omega(k) = \omega(k_0) + (k - k_0)\Big(\frac{d\omega}{dk}\Big)_0 + \cdots , \tag{45}$$

and the wave function can be written as

$$\psi(x, t) = \frac{A}{\sqrt{2\pi}}e^{i[k_0 x-\omega(k_0)t]}\int_{k_0-\frac{1}{2}\Delta k}^{k_0+\frac{1}{2}\Delta k} dke^{i(k-k_0)[x-(\frac{d\omega}{dk})_0 t]}$$

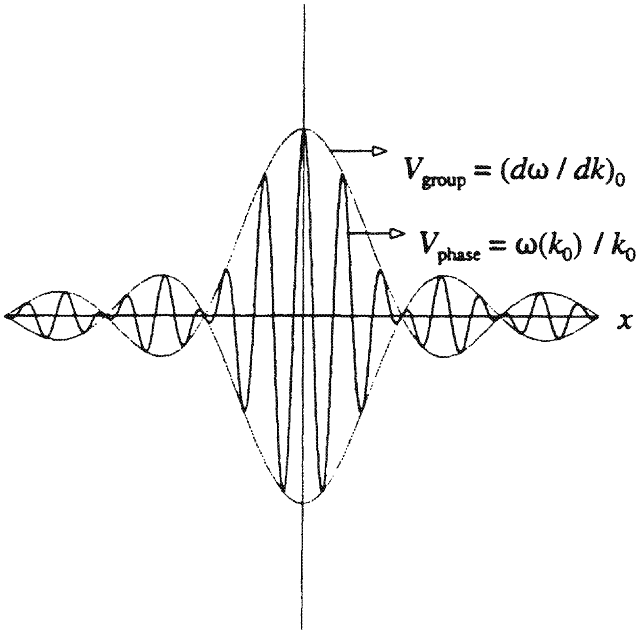

FIGURE 2.4. The wave packet of eq. (46).

$$= \sqrt{\frac{2}{\pi}} A e^{i[k_0 x - \omega(k_0)t]} \frac{\sin\left(\frac{\Delta k}{2}[x - (\frac{d\omega}{dk})_0 t]\right)}{[x - (\frac{d\omega}{dk})_0 t]}. \tag{46}$$

This wave packet is shown in Fig. 2.4. We note, in particular, the individual wavelets travel with the phase velocity

$$v_{\text{phase}} = \frac{\omega(k_0)}{k_0}. \tag{47}$$

The wave train itself, the envelope of the packet, however, travels with the group velocity

$$v_{\text{group}} = \left(\frac{d\omega}{dk}\right)_0. \tag{48}$$

If we assume most of the energy of the wave train lies in the large central peak of the wave envelope, we can take the extent of the wave packet to be $\Delta x \approx 2\frac{2\pi}{\Delta k}$. Even for more sophisticated functions, $A(k)$, we will find the Fourier integral analysis always gives

$$\Delta x \Delta k \approx 2\pi, \tag{49}$$

neglecting factors of order 2 in this approximation. This is the uncertainty relation for a wave packet. Note, in particular, it follows for all wave packets, merely from the Fourier analysis.

H Propagation of Wave Packets: The Wave Equation

The wave equation, the propagation law for the wave, is intimately related to the dispersion law

$$\omega = f(k). \tag{50}$$

In one dimension, with

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk A(k) e^{i(kx-\omega t)}, \tag{51}$$

$$-\frac{1}{i}\frac{\partial}{\partial t}\psi = \frac{1}{\sqrt{2\pi}}\int dk\omega A(k) e^{i(kx-\omega t)}, \tag{52}$$

$$\left(\frac{1}{i}\right)^n \frac{\partial^n}{\partial x^n}\psi = \frac{1}{\sqrt{2\pi}}\int dk k^n A(k) e^{i(kx-\omega t)}. \tag{53}$$

For functions $f(k)$ that can be given by Taylor expansions,

$$f(k) = \sum_{n=0} \alpha_n k^n,$$

we then have

$$f\left(\frac{1}{i}\frac{\partial}{\partial x}\right)\psi = \frac{1}{\sqrt{2\pi}}\int dk f(k) A(k) e^{i(kx-\omega t)}. \tag{54}$$

Eqs. (52) and (54) then lead to

$$\left[-\frac{1}{i}\frac{\partial}{\partial t} - f\left(\frac{1}{i}\frac{\partial}{\partial x}\right)\right]\psi = \frac{1}{\sqrt{2\pi}}\int dk[\omega - f(k)] A(k) e^{i(kx-\omega t)} = 0, \tag{55}$$

so the dispersion law, $\omega = f(k)$, leads to the wave equation

$$\left[-\frac{1}{i}\frac{\partial}{\partial t} - f\left(\frac{1}{i}\frac{\partial}{\partial x}\right)\right]\psi = 0. \tag{56}$$

For the special case of a nondispersive medium, with $\omega = ck$, we would have

$$-\frac{1}{i}\frac{\partial\psi}{\partial t} - \frac{c}{i}\frac{\partial\psi}{\partial x} = \int dk[\omega - ck] A(k) e^{i(kx-\omega t)} = 0. \tag{57}$$

So that, seemingly, the wave equation in this simple case of a nondispersive medium becomes

$$\frac{1}{c}\frac{\partial\psi}{\partial t} + \frac{\partial\psi}{\partial x} = 0. \tag{58}$$

This equation looks like a strange wave equation, however. Its solutions would be $\psi(x,t) = F(x-ct)$, where F is any arbitrary function. That is, this wave equation would permit wave propagation only in the positive x-direction and, hence, would correspond to a nonisotropic medium. The difficulty here is not with our method of arriving at the wave equation, but that we have written the dispersion law in a way that builds in this anisotropy. For a nondispersive, isotropic medium, we have to express the dispersion law in the form

$$\omega^2 - c^2k^2 = 0, \tag{59}$$

or in three dimensions

$$\omega^2 - c^2(k_x^2 + k_y^2 + k_z^2) = 0. \tag{60}$$

The technique we have used to arrive at the wave equation would then give us

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \frac{\partial^2\psi}{\partial x^2} = 0 \tag{61}$$

in one dimension, and

$$\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \nabla^2\psi = 0 \tag{62}$$

in three dimensions.

Note, finally, our method of arriving at the wave equation from the dispersion law is not a derivation of the wave equation. Our method may also not give a unique expression for the wave equation.