

# *Quantum Theory for the Computer Age Unit 3*



## *Fourier Analysis and Symmetry*

## Unit 3 Fourier Analysis and Symmetry

Unit 2 discussed quantum  $e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ -wave propagation in space and time and introduced wavevector and frequency  $(c\mathbf{k},\omega)$ -space while deriving the basic Einstein relativistic transformations and Planck-deBroglie quantum relations. But, what are  $e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$ -waves? One answer comes from understanding relations between space-time  $(\mathbf{x},ct)$  and  $(c\mathbf{k},\omega)$ -space known as Fourier transformations. Unit 3 begins with discussions of Fourier  $\langle \mathbb{X} | \mathbb{X} \rangle$  transformation matrices and shows their connection to translational symmetry. This with Planck's axiom gives the quantum equation of motion known as Schrodinger's time equation, the evolution operator, and its generator, the quantum Hamiltonian operator, the *sine qua non* of Schrodinger theory. Unit 3 continues with a detailed description of quantum beats and revivals using symmetry analysis. The final chapter describes 2-state and spin-1/2 systems while introducing U(2) symmetry analysis.

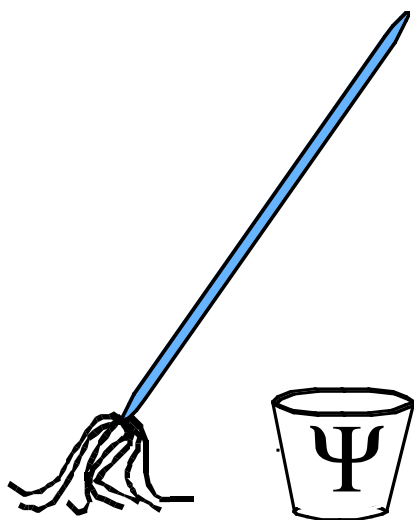
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# Unit 3 Fourier Analysis and Symmetry



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**W. G. Harter**

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Expressing arbitrary wavefunctions or states in terms of spectral components or plane waves is known as Fourier analysis. Fourier transformation matrices relate space and time (coordinate) bases to wavevector and frequency (Energy-momentum) bases of plane waves. Fourier analysis comes in different flavors depending on whether various bases are discretely numbered or continuous. Chapter 7 compares the continuous coordinate bases of Bohr rotor states to the fully continuous plane wave states of an unbounded continuum. Then a discrete “quantum-dot” system is introduced in which both coordinates and wavevectors are discrete. The later is the basis for the introduction of Fourier symmetry analysis in the following Chapter 8 and time evolution in Chapter 9. Discrete symmetry in space and time helps to clarify quantum beats and “revivals” which all quantum systems will exhibit to some degree.

## Unit 3 Fourier Analysis and Symmetry

### Chapter 7. Fourier Transformation Matrices

We have noted that a quantum experiment cannot move at all unless two or more frequency components can interfere with each other. A single (mono-chromatic) wave  $\Psi = \psi e^{-i\omega t}$  is not enough to make anything happen. Such a  $\Psi$ -system is a stationary state and appears to be dead. What we can observe is determined by the absolute square  $\Psi^*\Psi$ , which kills the single oscillating phase.

Similarly, a wave  $\Psi = \psi e^{ikx}$  with a single momentum component appears to be a uniform cloud of random counts in space. To obtain any structure in the quantum world, that is, atoms, molecules, solids, people, and so forth, we need *many* momentum components in our matter waves.

The mathematics used to deal with multiple frequency or momentum components is called *Fourier analysis* after Jean Baptiste Fourier, a French artillery officer turned mathematician. This section will review the fundamentals of Fourier theory relevant to quantum theory using the Dirac notation. Fourier analysis has several flavors depending on whether its coordinates and parameters, that is space-time and wavevector-frequency are discrete or continuous and whether  $x$  or  $k$  are bounded or unbounded. We consider several distinct cases in turn. Each has different forms for its completeness and orthonormality axioms-3 to 4.

#### 7.1 Continuous but bounded $x$ . Discrete but unbounded $k$

One of the most famous and widely used wavefunction systems in quantum theory are the one-dimensional (1-D) *Bohr orbitals*  $\psi_k(x) = \langle x | k \rangle$ . Examples are sketched in Fig. 7.1.1.

$$\psi_{k_m}(x) = \langle x | k_m \rangle = \frac{e^{ik_m x}}{\sqrt{\text{norm.}}} = \psi_{k_m}(x+L) \quad (7.1.1)$$

These can be thought of as a set of waves on a ring of circumference  $L$ . The basic waves have just the right wavevectors  $k_m$  to put integral numbers of whole wavelengths along  $L$  and thereby repeat the wave again after each complete  $L$ -revolution. Such requirements are known as *periodic boundary conditions*.

$$\psi_{k_m}(x) = \psi_{k_m}(x+L) = \frac{e^{ik_m x}}{\sqrt{\text{norm.}}} = \frac{e^{ik_m(x+L)}}{\sqrt{\text{norm.}}} = \psi_{k_m}(x) e^{ik_m L} \quad (7.1.2)$$

The boundary conditions lead to wavevector *quantization conditions*.

$$e^{ik_m L} = 1, \text{ or: } k_m = \frac{2\pi}{L} m, \text{ where: } m = 0, \pm 1, \pm 2, \pm 3, \dots, \pm \infty \quad (7.1.3)$$

The allowed wavevectors, while still infinite in number, are forced to be *discrete*.

This is a very common feature of quantum theory for which it owes its name *quantum*, but it happens to classical waves, too. A bounded continuum leads to an unbounded but discrete set of allowed waves. For another example, cavity modes in the Hall of Mirrors in Sec. 6.3 (d) acquire discrete frequencies as soon as the doors are shut. If an indiscrete type of wave is put in a cage, then it is forced to be discrete. (Perhaps, this is just another sad anthropomorphic metaphor.)

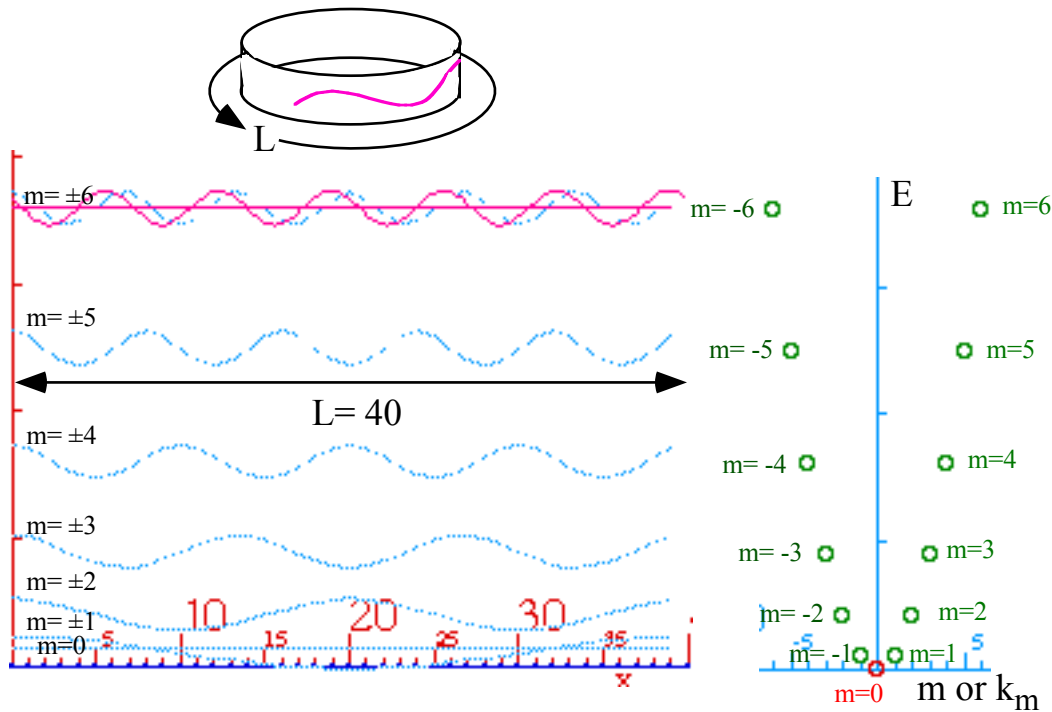


Fig. 7.1.1 Sketches of Bohr orbitals confined to 1-D  $L$ -interval and quantum energies (for  $m=0$  to 6).

The resulting amplitudes must satisfy Axioms 1-4. In particular, the orthonormality axiom-3 requires  $\langle k_1 | k_1 \rangle = 1$  but  $\langle k_1 | k_2 \rangle = 0$ , and so forth, or that the following Kronecker delta representation.

$$\langle k_m | k_n \rangle = \delta_{m n} \tag{7.1.4a}$$

Completeness axiom-4 requires that  $|k_n\rangle \langle k_n|$  sum up to a unit operator or an  $x$ -Dirac-delta expression.

$$\sum |k_n\rangle \langle k_n| = \mathbf{1}, \text{ or: } \sum \langle x | k_n \rangle \langle k_n | x' \rangle = \langle x | x' \rangle = \delta(x-x'). \tag{7.1.4b}$$

**(a) Orthonormality axiom-3**

Using the integral form (2.1.2) of the completeness relation sum we get the following.

$$\delta_{mn} = \langle k_m | k_n \rangle = \int_{-L/2}^{L/2} dx \langle k_m | x \rangle \langle x | k_n \rangle = \int_{-L/2}^{L/2} dx \frac{e^{-ik_m x}}{\sqrt{norm.}} \frac{e^{ik_n x}}{\sqrt{norm.}} \tag{7.1.5}$$

The conjugation axiom-2 was used to write

$$\langle k_m | x \rangle = \langle x | k_m \rangle^* = \frac{e^{-ik_m x}}{\sqrt{norm.}} \tag{7.1.6}$$

After integrating, this determines the *normalization constant*  $norm.$  as follows.

$$\begin{aligned} \delta_{mn} &= \int_{-L/2}^{L/2} dx \frac{e^{-ik_m x}}{\sqrt{norm.}} \frac{e^{ik_n x}}{\sqrt{norm.}} = \int_{-L/2}^{L/2} dx \frac{e^{-i(k_m - k_n)x}}{norm.} = \frac{e^{-i(k_m - k_n)L/2} - e^{-i(k_m - k_n)(-L/2)}}{-i(k_m - k_n)norm.} \\ &= \frac{e^{-i(k_m - k_n)L/2} - e^{i(k_m - k_n)L/2}}{-i(k_m - k_n)norm.} = \frac{2 \sin[(k_m - k_n)L/2]}{(k_m - k_n)norm.} \end{aligned} \tag{7.1.8}$$

Using the quantization conditions (7.1.3) gives the desired  $norm.$  value and satisfies axiom-3.

$$\delta_{mn} = \frac{2 \sin \pi(m-n)}{\frac{2\pi}{L}(m-n) \text{norm.}} = \begin{cases} 0 & \text{if: } m \neq n \\ \frac{L}{\text{norm.}} & \text{if: } m = n \end{cases}, \text{ or: } \text{norm.} = L. \quad (7.1.9)$$

Normalized wave amplitudes are therefore

$$\psi_{k_m}(x) = \langle x | k_m \rangle = \frac{e^{ik_m x}}{\sqrt{L}}. \quad (7.1.10)$$

### (b) Completeness axiom-4

Completeness axiom-4 has a Dirac-delta form in the mixed discrete-continuous wave space.

$$\delta(x-x') = \sum_{m=-\infty}^{m=+\infty} \langle x | k_m \rangle \langle k_m | x' \rangle \quad (7.1.11)$$

We test it with amplitudes (7.1.10) using orthonormality (7.1.4) and conjugation (7.1.5).

$$\int_{-L/2}^{L/2} dx \delta(x-x') = \int_{-L/2}^{L/2} dx \sum_{n=-\infty}^{n=+\infty} \frac{e^{ik_n x}}{\sqrt{L}} \frac{e^{-ik_n x'}}{\sqrt{L}} = \sum_{n=-\infty}^{n=+\infty} \frac{e^{-ik_n x'}}{\sqrt{L}} \int_{-L/2}^{L/2} dx \frac{e^{ik_n x}}{\sqrt{L}} \quad (7.1.12)$$

The last integral is a representation of a Kronecker delta  $\delta_{0,n}$ . Recall that  $k_0 = 0$  and use (7.1.4).

$$\begin{aligned} \int_{-L/2}^{L/2} dx \frac{e^{ik_n x}}{\sqrt{L}} &= \sqrt{L} \int_{-L/2}^{L/2} dx \frac{e^{-ik_0 x}}{\sqrt{L}} \frac{e^{ik_n x}}{\sqrt{L}} = \sqrt{L} \langle k_0 | k_n \rangle = \sqrt{L} \delta_{0,n} \\ \int_{-L/2}^{L/2} dx e^{ik_n x} &= L \delta_{0,n}. \end{aligned} \quad (7.1.13)$$

Then (7.1.12) is consistent with (7.1.11) and (7.1.10) and the definition of Dirac's delta.

$$\int_{-L/2}^{L/2} dx \delta(x-x') = \int_{-L/2}^{L/2} dx \sum_{n=-\infty}^{n=+\infty} \frac{e^{ik_n x}}{\sqrt{L}} \frac{e^{-ik_n x'}}{\sqrt{L}} = \sum_{n=-\infty}^{n=+\infty} e^{-ik_n x'} \delta_{0,n} = e^{-ik_0 x'} = 1 \quad (7.1.14)$$

### (c) Fourier series representation of a state

With completeness one can quickly derive a representation of arbitrary state  $|\Psi\rangle$  if you know its complex wavefunction  $\Psi(x) = \langle x | \Psi \rangle$ . Formally, you just operate on  $|\Psi\rangle$  with the unit  $\mathbf{1} = \sum |k_m\rangle \langle k_m|$ .

$$\begin{aligned} \langle x | \Psi \rangle &= \sum_{m=-\infty}^{m=+\infty} \langle x | k_m \rangle \langle k_m | \Psi \rangle = \sum_{m=-\infty}^{m=+\infty} \frac{e^{ik_m x}}{\sqrt{L}} \langle k_m | \Psi \rangle \\ &= \sum_{m=-\infty}^{m=+\infty} e^{ik_m x} \Psi_m \end{aligned} \quad (7.1.15a)$$

where the Fourier coefficient  $\Psi_m$  is given by the following integral (Use  $x$ -completeness  $\mathbf{1} = \int dx |x\rangle \langle x|$ .)

$$\begin{aligned} \Psi_m &= \frac{\langle k_m | \Psi \rangle}{\sqrt{L}} = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \langle k_m | x \rangle \langle x | \Psi \rangle = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dx \frac{e^{-ik_m x}}{\sqrt{L}} \langle x | \Psi \rangle \\ &= \frac{1}{L} \int_{-L/2}^{L/2} dx e^{-ik_m x} \Psi(x) \end{aligned} \quad (7.1.15b)$$

The only requirement is that the function be *periodic* in  $L$ , that is,  $\Psi(x) = \Psi(x+L)$ .

### (d) Bohr dispersion relation and energies

In Fig. 7.1.1 the waves with higher  $k_m$  have higher energy  $E_m$  and are drawn higher according to the  $E$ -values given by the *Bohr dispersion function* first drawn in Fig. 5.6.3.



$$E_m = \hbar\omega_m = \frac{(\hbar k_m)^2}{2M}, \text{ where: } p_m = \hbar k_m = \hbar \frac{2\pi}{L} m. \quad (7.1.16)$$

This is just a non-relativistic approximation for energy that neglects the rest energy  $Mc^2$  and higher order terms in (5.2.5b). It is kinetic energy only, that is  $KE = 1/2Mu^2 = p^2/2M$  with the momentum  $p=p_m$  and wavevector  $k=k_m$  quantized by conditions (7.1.3). The dispersion function is then a simple parabola of discrete values as shown on the right hand side of Fig. 7.1.1. Note that each energy value  $E_m$ , except  $E_0$ , has two orthogonal wavefunctions  $\psi_{\pm k_m}$  or states  $|\pm k_m\rangle$  corresponding to pairs of oppositely moving wavevectors  $\pm k_m$  on either side of the dispersion parabola. The  $|\pm k_m\rangle$  are called *degenerate states* because they share a single energy  $E_m$ . Such degenerate pairs are each an example of a U(2) two-state system. As long as the degeneracy remains, any unitary linear combination of the two states is also an eigenstate with the same frequency and energy  $E=h\nu$ .

### (e) Sine and cosine Fourier series worth remembering

A function defined by Fourier series (7.1.15) repeats after its fundamental wavelength  $L=2\pi/k_1$  or period  $T=2\pi/\omega_1$ . So do the real and imaginary parts that are series of sine or cosine functions of  $m^{\text{th}}$  spatial overtone argument  $k_mx$  or  $m^{\text{th}}$  overtone frequency argument  $\omega_mt$ . Moving wave terms use both:  $(k_mx - \omega_mt)$ .

Let us consider wave functions with *zero-DC-bias* or zero ( $k=0$ )-Fourier component:  $0=\Psi_0=\int\Psi$ . The integrals and derivatives of unbiased functions may also be unbiased. An example of a series of unbiased functions starts with the *alternating Dirac delta function adel(x)* shown at the top of Fig. 7.1.2. Its integrals and derivatives are useful series worth remembering because they are easy to compute and visualize. Compare this function to the simple delta pulse train (5.3.2) shown in Fig. 5.3.2.

The first integral of *adel(x)* is a *square wave function box(x)* shown next in line in Fig. 7.1.2. Below it is a *saw-tooth wave saw(x)* and then a *parabolic amplitude wave paw(x)*. Each wave has an overall scale factor attached so plots that are not delta-like end up with comparable amplitudes.

Wave *paw(x)* looks like a sine wave but isn't quite. The derivative of a genuine sine wave is a cosine wave that looks just like a sine wave but is moved back by  $\pi/2$ . The derivative of *paw(x)* is *saw(x)*, which is moved back, but it looks nothing like good old *paw(x)*! Subsequent derivatives only accentuate the differences between *sin(x)* and *paw(x)*. Differentiation amplifies little blips or bends (It differentiates!) while integration does the opposite by smoothing out sharp corners or other differences.

There are at least two famous physics topics that make use of functions that are derivatives or integrals of each other. Classical mechanics in one dimension is one such topic where the functions of *acceleration a(t)*, *velocity v(t)*, and *position x(t)*, are each the integral of one above or the derivative of the one below. Classical electrostatics is another topic in which the *charge-density ρ(x)*, *electric field E(x)*, and *potential Φ(x)*, are so related. (Various conventions may put  $\pm$  signs and scale factors onto these relations.)

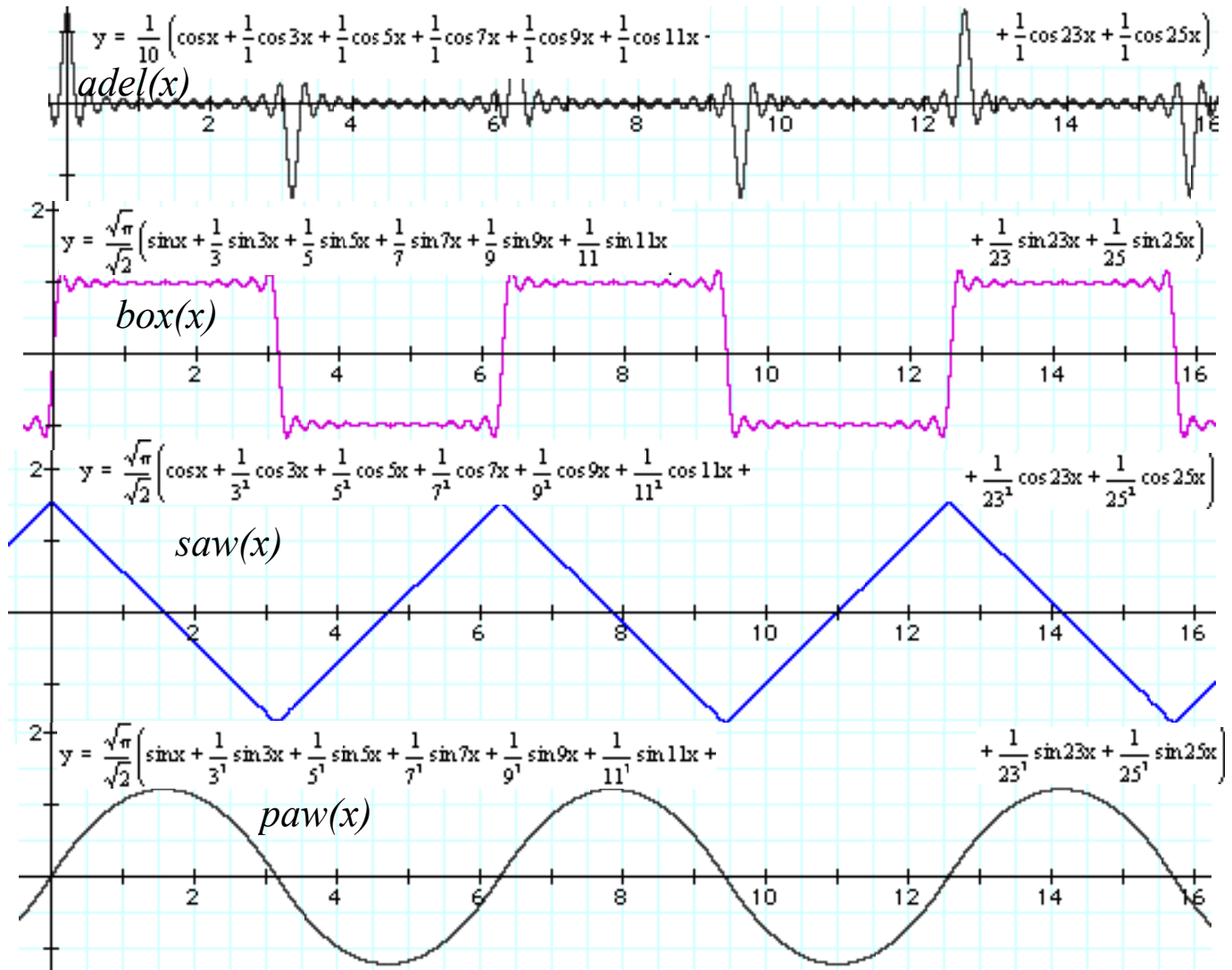
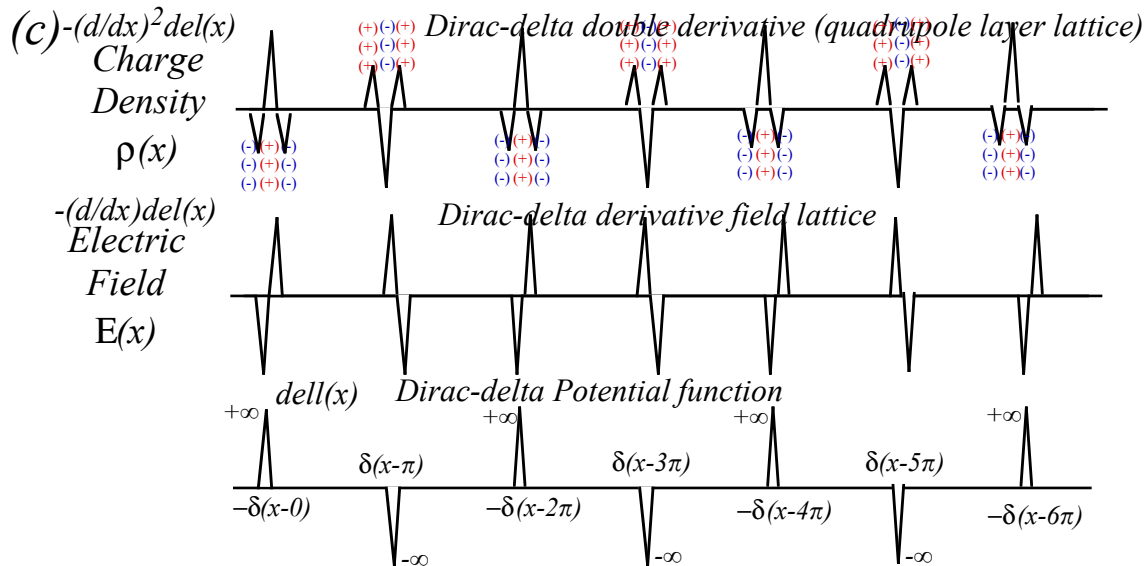
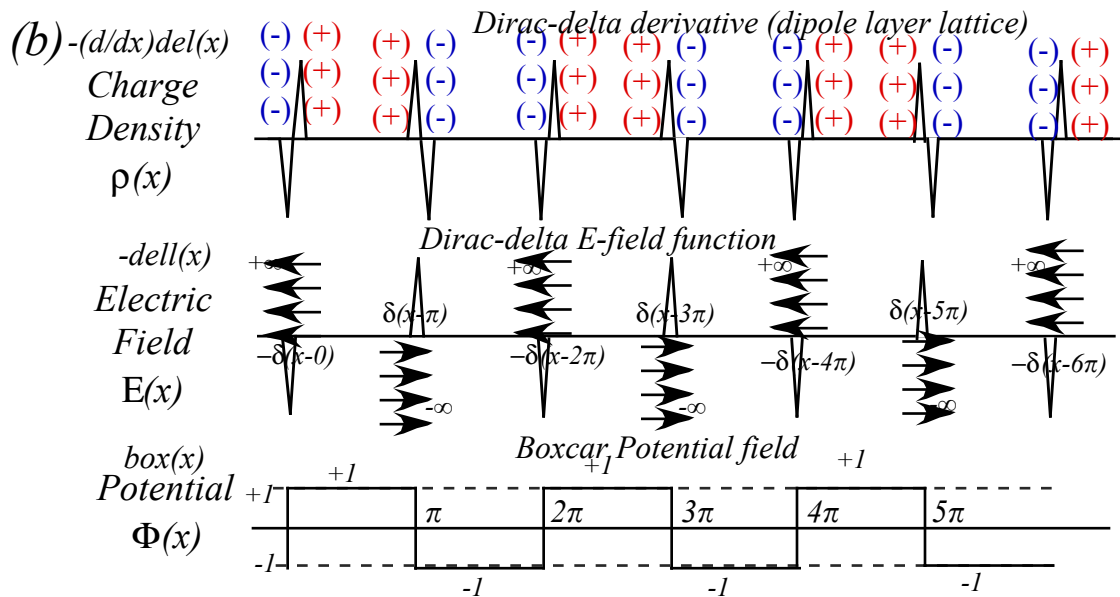
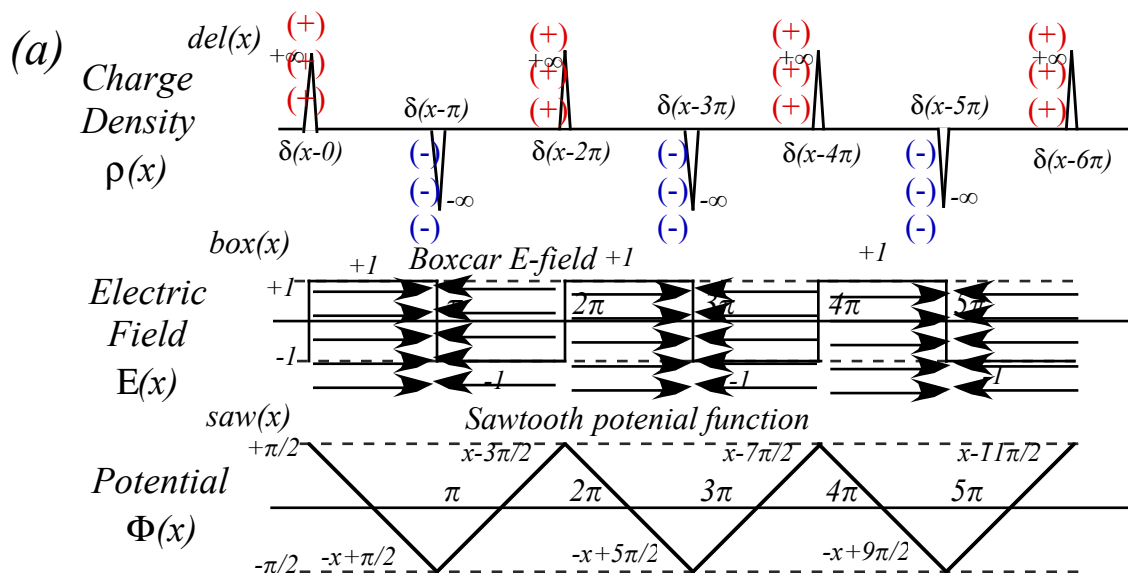


Fig. 7.1.2 Fourier series sharing simple integral or derivative relations to each other.

Some more or less extreme examples of charge and field distributions are sketched in Fig. 7.1.3 on the following page. The first set in Fig. 7.1.3(a) is due to alternating charge layers. The field is that of a series of alternating parallel-plate capacitors. By taking a derivative of the alternating charge layers we make the dipole layer distribution shown in the top of the middle Fig. 7.1.3(b). The final example in Fig. 7.1.3(c) actually has a Dirac-delta potential lattice, one of many favorite models for nano science these days. We shall be modeling periodic potentials, too. The preceding gives you some feeling how difficult it may be to actually *produce* some of these exotic potentials! Seldom is theory so easy and the lab so hard.

Also it is worth considering these as time-pulse series. As we will explain later, you may taper the Fourier series amplitudes gradually to zero and thereby replace the sharp and wrinkled deltas and squares by smoother Gaussian or Lorentzian features that are useful spectroscopic models. Of course, you may taper them right back to single term series of one sine or one cosine wave each!

Following page: Fig. 7.1.3 Exotic 1-D electric charge and field distributions.



## 7.2 Continuous and unbounded $x$ . Continuous and unbounded $k$

In the preceding cases all wavevectors are restricted by the quantization condition (7.1.3).

$$k_m = \frac{2\pi}{L} m, \text{ where: } m = 0, \pm 1, \pm 2, \pm 3, \dots, \pm \infty \quad (7.1.3)_{\text{repeated}}$$

If you let the "cage" become infinitely large ( $L \rightarrow \infty$ ) then the wavevector set becomes finer and finer and approaches a *continuum*. The trick is to replace each sum over index  $m$  by an integral over a continuous  $k$ -value. If it is done right the wave functions will take a continuous form in *both*  $x$  and  $k$ .

$$\psi_k(x) = \langle x | k \rangle = \frac{e^{ikx}}{\sqrt{\text{norm.}}} , \quad (7.2.1a)$$

We need to verify  $k$ -orthonormality relations based on wavevector Dirac-delta  $\delta(k', k)$ -functions.

$$\langle k' | k \rangle = \delta(k' - k) = \int_{-\infty}^{\infty} dx \langle k' | x \rangle \langle x | k \rangle = \int_{-\infty}^{\infty} dx \psi_{k'}(x)^* \psi_k(x) , \quad (7.2.1b)$$

We also need the usual  $x$ -completeness relations based on spatial Dirac-delta  $\delta(x', x)$ -functions.

$$\langle x' | x \rangle = \delta(x' - x) = \int_{-\infty}^{\infty} dk \langle x' | k \rangle \langle k | x \rangle = \int_{-\infty}^{\infty} dk \psi_k(x')^* \psi_k(x) \quad (7.2.1c)$$

It seems that orthonormality and completeness relations are two sides of the same coin. Orthonormality (7.2.1b) for the  $k$ -states  $\{|k\rangle \dots |k'\rangle \dots\}$  expresses completeness for the  $x$ -states  $|x\rangle$ , and completeness (7.2.1c) of the  $k$ -states  $|k\rangle$  expresses orthonormality for the  $x$ -states  $\{|x\rangle \dots |x'\rangle \dots\}$ .

The Dirac notation is extremely efficient but can be confusing. There is a world of difference between the states  $\{|k\rangle \dots |k'\rangle \dots\}$  of perfectly monochromatic plane waves and the Dirac position states  $\{|x\rangle \dots |x'\rangle \dots\}$  of perfectly localized particles. Recall that we said that an  $|x\rangle$  state was physically unrealizable; crushing a particle into a single position- $x$  would cost infinite energy. Technically, a  $|k\rangle$  state is unrealizable, too, since it requires an infinite amount of real estate; we have to let its cage dimension  $L$  be infinite, but that seems easier than the extreme solitary confinement needed to make an  $|x\rangle$  state. If space is cheaper than energy, then  $|k\rangle$  is easier to approach than  $|x\rangle$ . Lasers easily make approximate  $|k\rangle$ 's by being stable and coherent, but producing approximate  $|x\rangle$ 's for extremely short pulses requires more difficult engineering.

Use caution to not abuse this notation, though it is easily done. It should be obvious why the following rendition of (7.2.1a) is a dreadful mistake.

$$\langle k | k \rangle = \frac{e^{i k k}}{\sqrt{\text{norm.}}} = \frac{e^{i k^2}}{\sqrt{\text{norm.}}} \quad (\text{Dirac abuse. Very BAD mistake!})$$

Letters  $x$  and  $k$  denote very different bases which must not to be confused.

### (a) Fourier integral transforms

To achieve the limit of infinite real estate ( $L \rightarrow \infty$ ) we replace sums over  $k_m = \frac{2\pi}{L} m$  such as

$$S = \sum_{m=-\infty}^{m=+\infty} \Phi_{k_m} = \sum_{m=-\infty}^{m=+\infty} \Delta m \Phi_{k_m}, \text{ where: } \Delta m = 1 . \quad (7.2.2)$$

Integrals over  $k$  with differential  $\Delta k_m = \frac{2\pi}{L} \Delta m = \frac{2\pi}{L} \rightarrow dk$  or:  $\frac{\Delta m}{\Delta k_m} = \frac{L}{2\pi}$  are used as follows.

$$S = \sum_{m=-\infty}^{m=+\infty} \Delta m \Phi_{k_m} = \sum_{m=-\infty}^{m=+\infty} \frac{\Delta m}{\Delta k_m} \Delta k_m \Phi_{k_m} \text{ becomes } \rightarrow \frac{L}{2\pi} \int_{-\infty}^{+\infty} dk \Phi(k) \quad (7.2.3)$$

This, by itself, blows up as we let  $(L \rightarrow \infty)$ , but so do the normalization denominators  $\sqrt{norm.} = \sqrt{L}$ , and they cancel. Finally, the Fourier series (7.1.15a) becomes a finite integral.

$$\langle x | \Psi \rangle = \sum_{m=-\infty}^{m=+\infty} \frac{e^{ik_m x}}{\sqrt{L}} \langle k_m | \Psi \rangle \text{ becomes } \rightarrow \frac{L}{2\pi} \int_{-\infty}^{+\infty} dk \frac{e^{ikx}}{\sqrt{L}} \langle k_m | \Psi \rangle = \int_{-\infty}^{+\infty} dk \frac{e^{ikx}}{\sqrt{2\pi}} \frac{\sqrt{L}}{\sqrt{2\pi}} \langle k_m | \Psi \rangle$$

The trick is to renormalize the  $k$ -bases so  $\frac{\sqrt{L}}{\sqrt{2\pi}} \langle k_m |$  becomes  $\langle k |$  letting the  $L$ 's cancel.

$$\langle x | \Psi \rangle = \int_{-\infty}^{+\infty} dk \frac{e^{ikx}}{\sqrt{2\pi}} \langle k | \Psi \rangle = \int_{-\infty}^{+\infty} dk \langle x | k \rangle \langle k | \Psi \rangle, \quad (7.2.4a)$$

The newly “normalized” plane wave function  $\psi_k(x) = \langle x | k \rangle$  is defined as follows.

$$\langle x | k \rangle = \frac{e^{ikx}}{\sqrt{2\pi}} \quad (7.2.4b)$$

This  $\langle x | k \rangle$  is the *kernel* of a *Fourier integral transform*. An inverse follows by converting (7.1.15b).

$$\frac{\langle k_m | \Psi \rangle}{\sqrt{L}} = \frac{1}{L} \int_{-L/2}^{L/2} dx e^{-ik_m x} \langle x | \Psi \rangle \text{ becomes } \rightarrow \langle k | \Psi \rangle = \frac{\sqrt{L}}{\sqrt{2\pi}} \frac{\sqrt{L}}{L} \int_{-\infty}^{+\infty} dx e^{-ikx} \langle x | \Psi \rangle,$$

$$\langle k | \Psi \rangle = \int_{-\infty}^{+\infty} dx \frac{e^{-ikx}}{\sqrt{2\pi}} \langle x | \Psi \rangle = \int_{-\infty}^{+\infty} dx \langle k | x \rangle \langle x | \Psi \rangle, \quad (7.2.4c)$$

Here the *inverse kernel*  $\langle k | x \rangle$  is simply the conjugate of  $\langle x | k \rangle$  as required by conjugation axiom-2.

$$\langle k | x \rangle = \frac{e^{-ikx}}{\sqrt{2\pi}} = \langle x | k \rangle^*. \quad (7.2.4d)$$

**(b) Fourier coefficients: Their many names**

The efficiency of the Dirac notation (provided it isn't abused!) should be clear by now. The simple bra-ket  $\langle x | k \rangle$  stands for so many different mathematical and physical objects. Let's list some.

- (1)  $\langle x | k \rangle$  is a *scalar product* of bra  $\langle x |$  and ket  $| k \rangle$
- (2)  $\langle x | k \rangle$  is an *x-wavefunction* for a state  $| k \rangle$  of definite momentum  $p = \hbar k$ .
- (3)  $\langle k | x \rangle = \langle x | k \rangle^*$  is a *k-wavefunction* for a state  $| x \rangle$  of definite position  $x$ .
- (4)  $\langle x | k \rangle$  is a unitary *transformation matrix* from position states to momentum states.
- (5)  $\langle x | k \rangle$  is the *kernel* of a Fourier transform between position states and momentum states.

As beautiful and compact as it is, the continuum functional Fourier analysis is merely an infinite and unbounded abstraction that lets us use calculus to derive formulas in special cases. Its validity as a limiting case for experimental and numerical analysis should always be questioned. Laboratory and computer experiments, on the other hand, invariably deal with finite and bounded spaces, and it these that we turn to in the next section. We finish this section by relating square-wave Fourier transforms to square-wave Fourier series of the preceding section to help clarify discrete-vs.-continuum relations.

### (c) Time: Fourier transforms worth remembering

Fourier time-frequency (time-per-time) transforms resemble space- $k$ -vector (space-per-space) transforms (7.2.4). But, a negative sign is put in the exponent so the time phasor turns clockwise.

$$\langle t | \Psi \rangle = \int_{-\infty}^{+\infty} d\omega \frac{e^{-i\omega t}}{\sqrt{2\pi}} \langle \omega | \Psi \rangle = \int_{-\infty}^{+\infty} d\omega \langle x | \omega \rangle \langle \omega | \Psi \rangle \quad (7.2.5a) \quad \langle t | \omega \rangle = \frac{e^{-i\omega t}}{\sqrt{2\pi}} \quad (7.2.5b)$$

$$\langle \omega | \Psi \rangle = \int_{-\infty}^{+\infty} dt \frac{e^{i\omega t}}{\sqrt{2\pi}} \langle t | \Psi \rangle = \int_{-\infty}^{+\infty} dt \langle \omega | t \rangle \langle t | \Psi \rangle \quad (7.2.5c) \quad \langle \omega | t \rangle = \frac{e^{i\omega t}}{\sqrt{2\pi}} = \langle t | \omega \rangle^*$$

Consider, for example, a single square bump of amplitude  $B$  and duration  $T/2$ . Its Fourier transform (7.2.5c) is an *elementary diffraction function*  $\sin \omega/\omega$  that is plotted in Fig. 7.2.1.

$$\langle \omega | \Psi \rangle = \int_{-T/4}^{+T/4} dt \frac{e^{i\omega t}}{\sqrt{2\pi}} B = B \frac{e^{i\omega T/4} - e^{-i\omega T/4}}{i\omega\sqrt{2\pi}} = \frac{2B \sin(\omega T/4)}{\omega\sqrt{2\pi}} \quad (7.2.6)$$

It is the first approximation to an optical diffraction function for a single square aperture.

The Fourier amplitude due to multiple square humps is a combination of finer and finer elementary diffraction patterns. Three half-humps give the following frequency function plotted in Fig. 7.2.2(a).

$$\begin{aligned} \langle \omega | \Psi \rangle &= \frac{1}{\sqrt{2\pi}} \left[ A \int_{-3T/4}^{-T/4} dt e^{i\omega t} + B \int_{-T/4}^{+T/4} dt e^{i\omega t} + A \int_{+T/4}^{+3T/4} dt e^{i\omega t} \right] \\ &= A \frac{e^{-i\omega T/4} - e^{i3\omega T/4}}{i\omega\sqrt{2\pi}} + B \frac{e^{i\omega T/4} - e^{-i\omega T/4}}{i\omega\sqrt{2\pi}} + A \frac{e^{i3\omega T/4} - e^{i\omega T/4}}{i\omega\sqrt{2\pi}} \quad (7.2.7) \\ &= \frac{2(B-A)\sin(\omega T/4)}{\omega\sqrt{2\pi}} + \frac{2A\sin(3\omega T/4)}{\omega\sqrt{2\pi}} \end{aligned}$$

The frequency functions in Fig. 7.2.3 are the result of a lot more bumps. Each one consists of a series of spikes corresponding to the Fourier series amplitudes  $1, 1/3, 1/5, 1/7, \dots$  for the fundamental  $\omega=2\pi/T$  and odd-overtones  $3\omega, 5\omega, 7\omega, \dots$ , respectively, for the *box(x)* function in Fig. 7.1.2. This is an even box function in Fig. 7.2.3 so the series amplitudes alternate sign as  $1, -1/3, 1/5, -1/7, \dots$  as shown. The very last example is an unbiased function with no DC ( $\omega=0$ )-Fourier component.

The "ringing" between the peaks is generally considered to be a nuisance. One way to get rid of ringing is to turn on the square wave more gradually. Fig. 7.2.4 shows the Fourier transform of a wave that has been turned on and off by a Gaussian ( $\exp(-x/a)^2$ ). This *windowing* kills the ringing. The width of each frequency peak varies inversely with the width  $a$  of the Gaussian window.

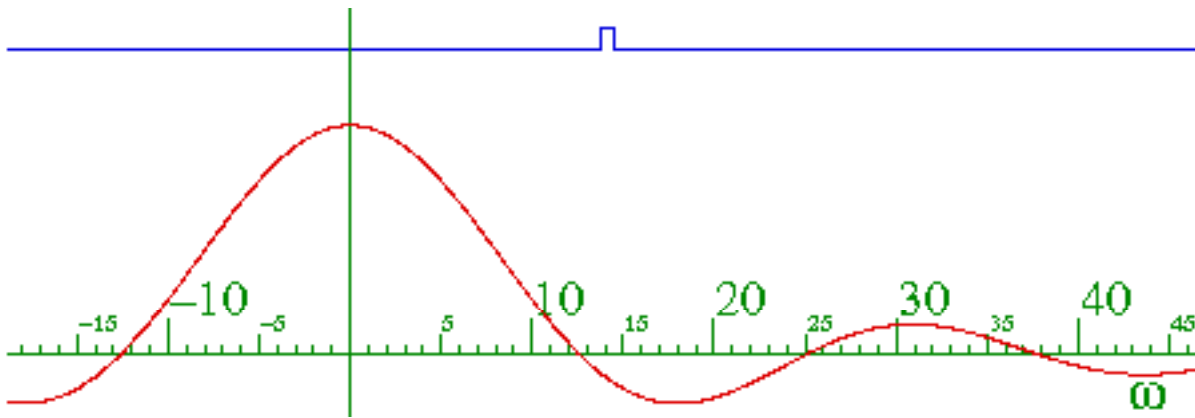


Fig.7.2.1 Elementary diffraction function: Fourier transform of single half square wave.

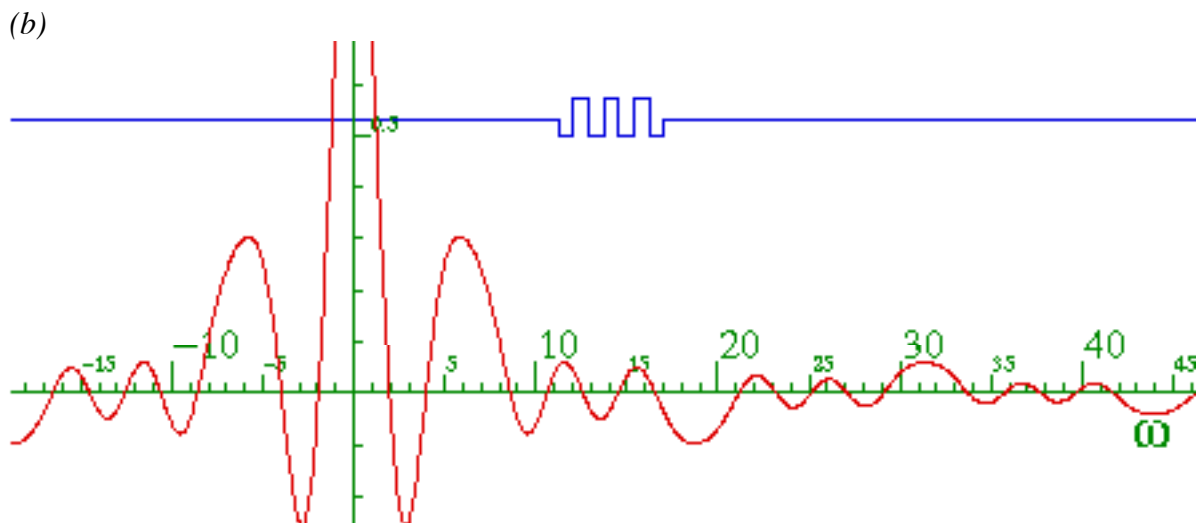
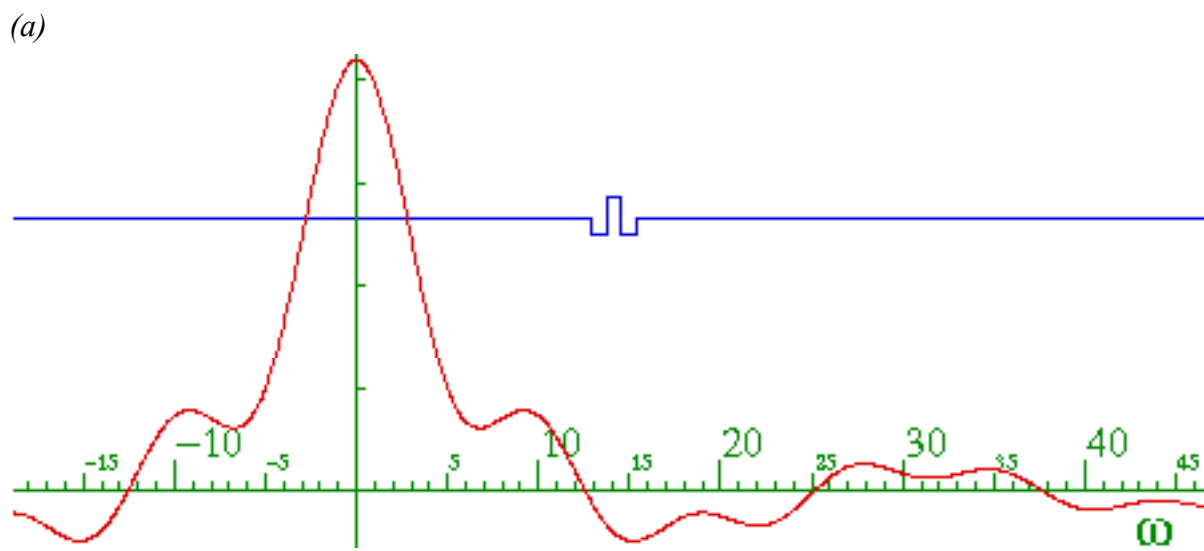
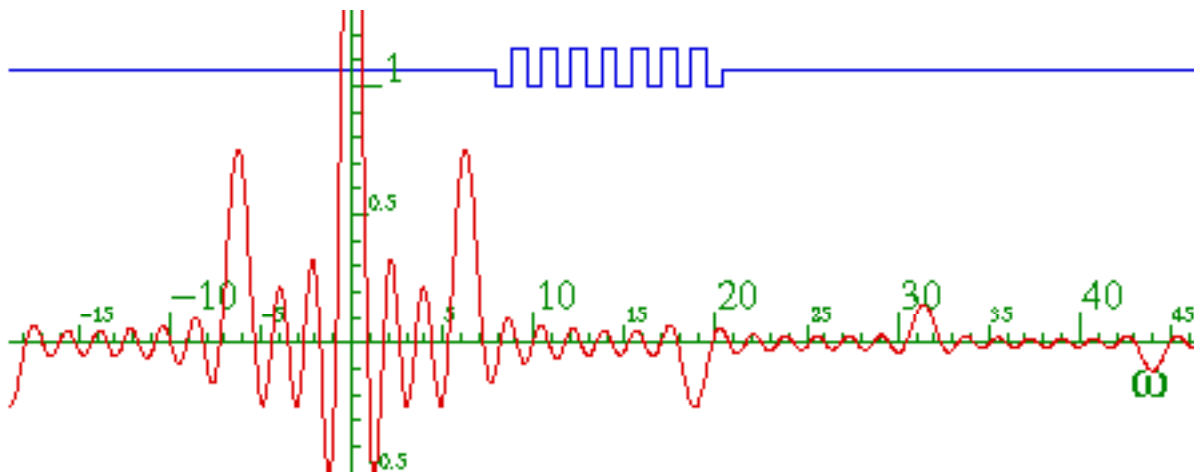
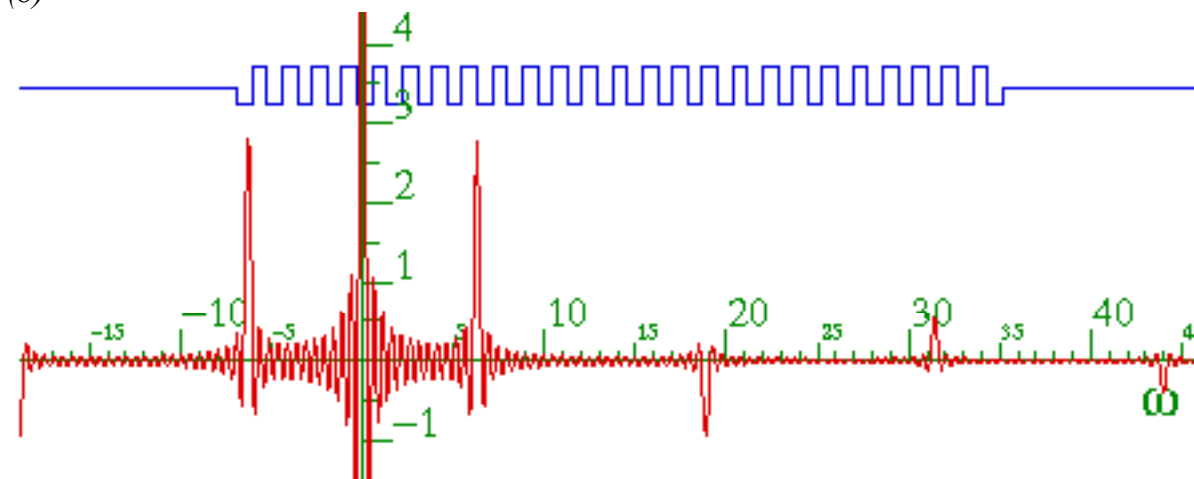


Fig. 7.2.2 Fourier transform of (a) three half- square waves. (b) seven half-square waves.

(a)



(b)



(c)

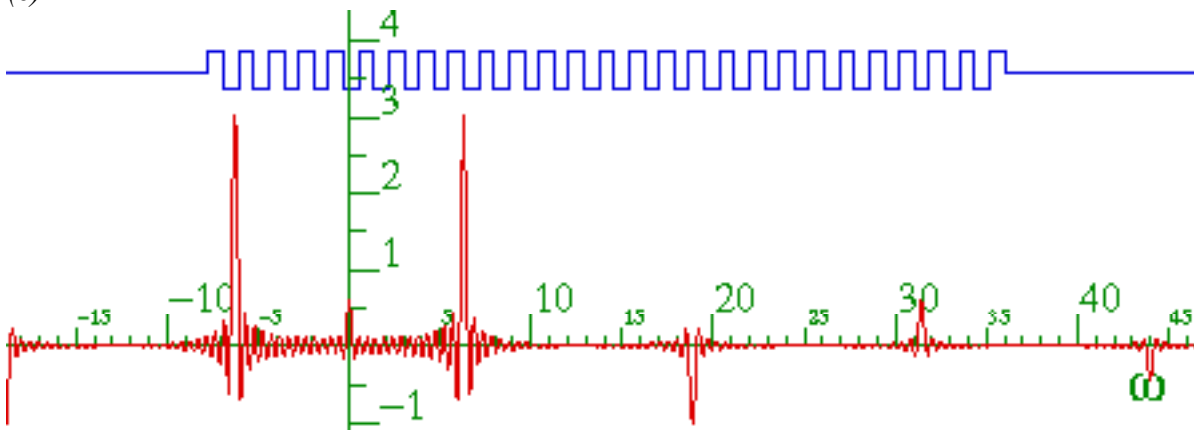


Fig. 7.2.3 Fourier transforms of square half-bumps (a) fifteen (b) forty-nine (c) fifty one .



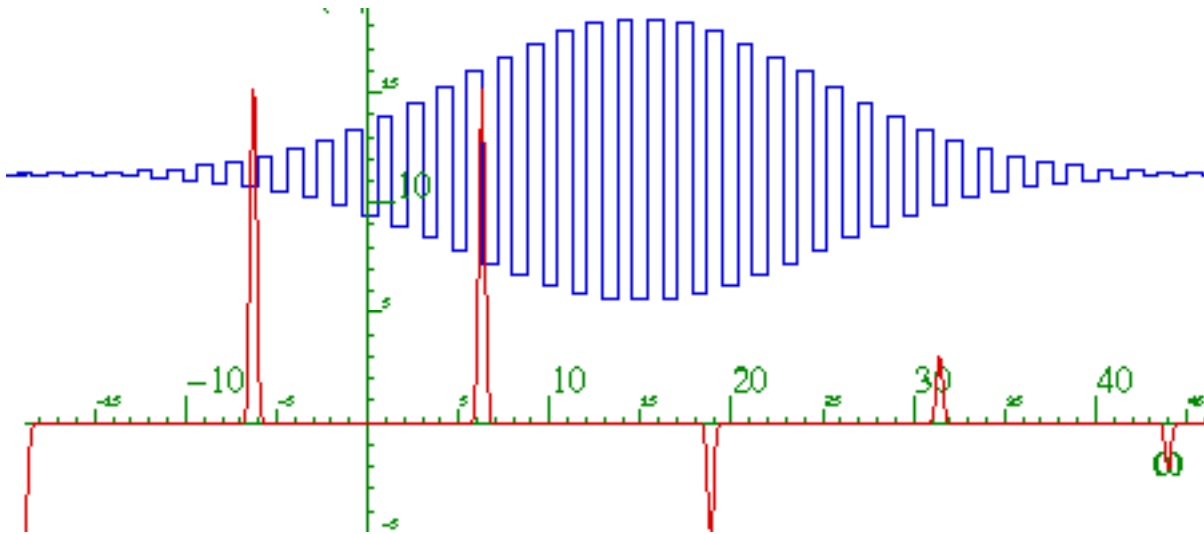


Fig. 7.2.4 Fourier transform of windowed square waves.

The idea of the Fourier integral, as opposed to Fourier series, is that any function, periodic or otherwise can be approximated by sines and cosines from a frequency *continuum*. Fourier series require that the function be periodic and repeat itself perfectly after some fixed period of time. The Fourier integral is supposed to be an enduring and time-invariant frequency map that provides the predestination of a time function forever and ever!

One should be suspicious of something that requires an infinite continuum of perfect frequency oscillators to be behind the scenes running your life. Pure sines and cosines are forever functions but we, like our world, certainly are not so enduring. Consider Fourier integrals as a cute limit-taking tool but not ultimately realistic.

Consider the fictitious function of time shown in Fig. 2.6.6. It is only periodic for awhile, but like most of us, cannot maintain the pace forever and finally gets in trouble with the hereafter.

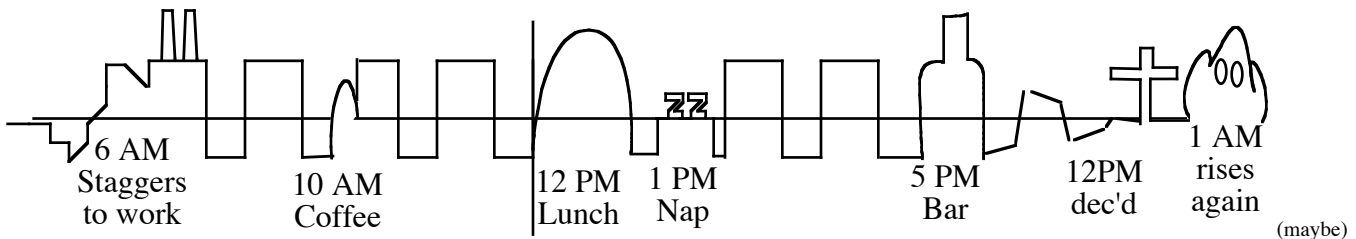


Fig. 7.2.5 A day in the life of a real function.

Now we go on to a practical Fourier analysis that is both finite and discrete.

### 7.3 Discrete and bounded $x$ . Discrete and bounded $k$

This is the most restrictive case, but also, due to practical considerations mentioned previously, the one that actually gets used the most these days. However, in spite of its practical value it is not always treated as carefully as the more “mathematically sophisticated” continuum case (b). It should be!

We begin by supposing that space itself is periodic as in case (a) but further is divided into  $N$  discrete pieces or points. So the only  $x$ -values allowed are the following  $N$  values

$$\{ x_0=0, x_1=a, x_2=2a, x_3=3a, \dots, x_{N-1}=(N-1)a, x_N=0 \} \tag{7.3.1a}$$

and there are only  $N$  position states are the following. The last  $|N\rangle$  state is the same as the first  $|0\rangle$  state.

$$\{ |0\rangle, |1\rangle, |2\rangle, |3\rangle, \dots, |N-1\rangle, |N\rangle=|0\rangle \} \tag{7.3.1b}$$

Fig. 7.3.1 shows ways to visualize this as  $N$  beads on a ring of length  $L = Na$  that wraps around so that the  $N$ -th bead is the same as the *zero*-th. (Zero-based numbering is the modern computing standard.) Otherwise, we invoke the so-called *periodic* or *Born-VonKarman* boundary conditions and imagine our 1-D world repeats like a computer game outside its boundaries. As shown in Fig. 7.3.1, there is a distance  $a$  between the lattice of beads. It is called the *lattice spacing*  $a$ .

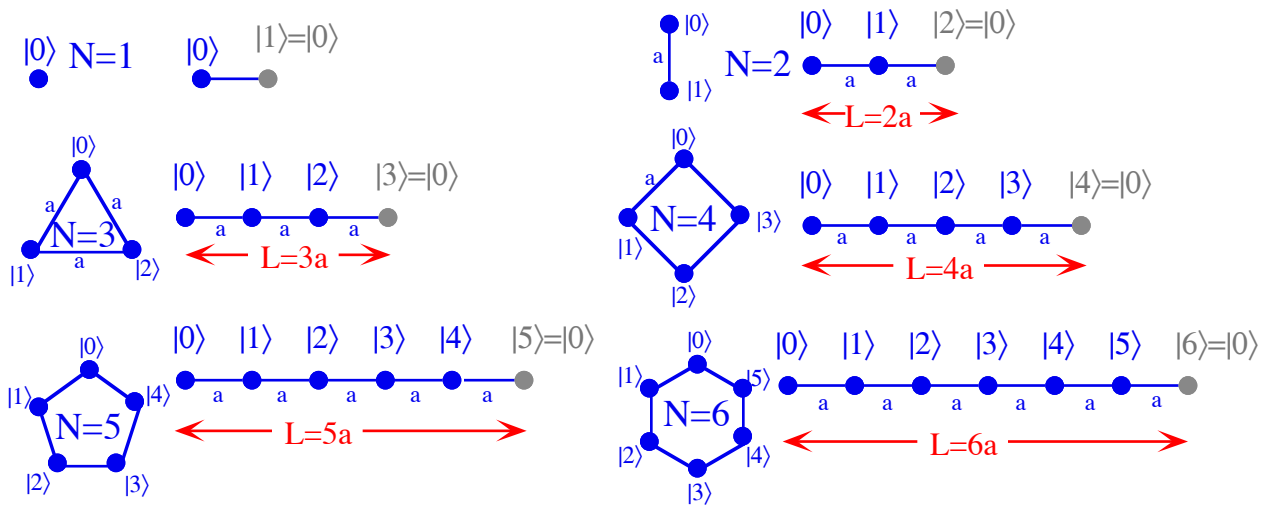


Fig. 7.3.1 Finite coordinate spaces for  $N$ -cyclic ( $C_N$ ) discrete systems ( $N = 1, 2, \dots, 6\dots$ )

These *ideal quantum dots* will be among our first examples of 2-state, 3-state, ..., and 6-state systems. By studying them carefully, it will be possible to learn important principles which will greatly help later study of molecules and solids which have  $N$ -states with large- $N$  but the same basic theory. Also, the quantum dots might have hidden inventions that could make you wealthy!

The basic wavefunctions that live on the discrete dots or beads are a subset of the continuum wavefunctions  $e^{ikmx}$  of (2.6.1), as though  $N$  equally spaced points of (2.6.1) were extracted and plotted over each lattice point  $x_p$  where

$$x_p = p a = p L/N \quad ( p = 0, 1, 2, 3, \dots, N-1 ) \tag{7.3.2}$$

The basic wavefunctions are given explicitly below.

$$\psi_{k_m}(x_p) = \langle x_p | k_m \rangle = \frac{e^{ik_m x_p}}{\sqrt{N}} = \psi_{k_m}(x_p + L) \tag{7.3.3}$$

The only change from (7.1.1) is the use of a discrete coordinate  $x_p$  defined in (7.3.2) above. Also, the normalization constant has been set to the dimension  $N$  since all  $N$  exponentials  $e^{ik_m x}$  contribute unit magnitude ( $|e^{ik_m x}|^2 = 1$ ) in the normalization sum.

$$\langle k_m | k_m \rangle = \sum_{p=0}^{N-1} \langle k_m | x_p \rangle \langle x_p | k_m \rangle = \sum_{p=0}^{N-1} \frac{e^{-ik_m x_p}}{\sqrt{N}} \frac{e^{ik_m x_p}}{\sqrt{N}} = N \frac{1}{\sqrt{N}} \frac{1}{\sqrt{N}} = 1 \tag{7.3.4}$$

The quantization conditions due to periodicity requirement (7.3.3) over "cage" length  $L=Na$  are similar to (7.1.3) but now expressed in terms of the discrete number  $N$  and spacing  $a$  of lattice points.

$$e^{ik_m L} = 1, \text{ or: } k_m = \frac{2\pi}{L} m = \frac{2\pi}{Na} m \tag{7.3.5a}$$

Wave amplitude at lattice point  $p$  is a power- $p$  of  $(e^{i2\pi/N})$ , the  $N$ -th root of unity (normalized, of course)

$$\psi_{k_m}(x_p) = \langle x_p | k_m \rangle = \frac{e^{ik_m x_p}}{\sqrt{N}} = \frac{1}{\sqrt{N}} \left( e^{i2\pi/N} \right)^{mp} \tag{7.3.5b}$$

All  $N$  roots, together, form  $N$ -polygons in the complex plane as shown in Fig. 7.3.2. The allowed wave amplitudes in Fig. 7.3.2 resemble the "ring" coordinate positions in Fig. 7.3.1. The complex  $z_{m,p} = \exp(ik_m x_p)$  are the  $N$ -th roots of unity ( $z^N = 1$ ) introduced in a complex arithmetic review (App 1.A).

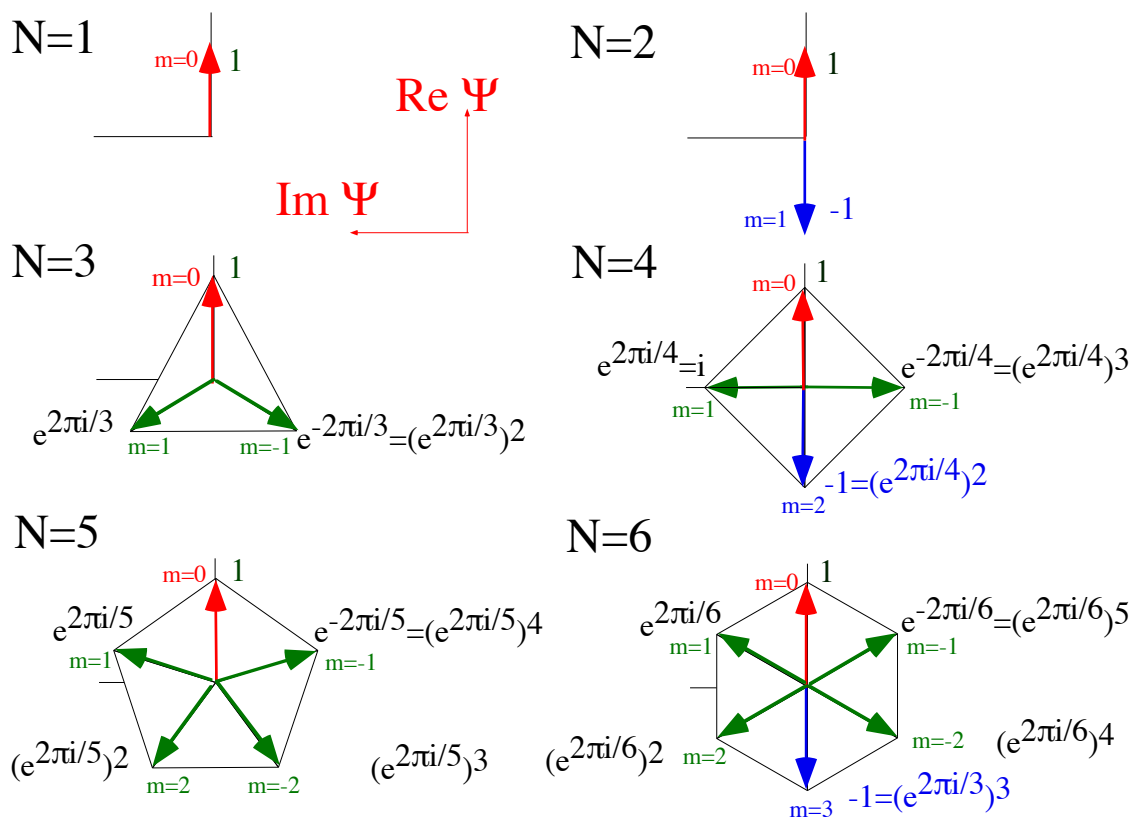


Fig. 7.3.2 Discrete wave amplitudes allowed for  $N$ -cyclic ( $C_N$ ) systems ( $N = 1, 2, \dots, 6, \dots$ )

### (a) N-nary counting for N-state systems

Fig. 7.3.2 shows different counting schemes for *odd-N* and *even-N*. In the unbounded cases the  $k$ -values go from  $-\infty$  to  $+\infty$ . Here, letting  $m$  count from  $-N$  to  $+N$  over-counts and gives  $2N+1$  states when we know there are only  $N$ . We could let  $m$  count from  $0$  to  $N-1$ , just like the lattice points. Or, we let  $m$  count from  $-(N-1)/2$  to  $+(N-1)/2$ , (*odd-N*) and from  $-(N-2)/2$  to  $+(N)/2$  (*even-N*) as shown below.

It helps to think of  $N$ -state cyclic system as an *N-nary* computer element. Ever since 1950, we have become accustomed to binary ( $N=2$ ) data storage in 2-bit registers. Inevitably, someone will discover how to make  $N$ -state registers. Until then, we imagine them. For an  $N$ -state register the quantum counting index  $m$  is defined only by an *integer modulo-N* or  $(m)_N$ .

$$(m)_N = m \text{ modulo } N \quad (7.3.6)$$

For example, for  $N=6$  in Fig. 7.3.2, all the following values of the quantum index  $m$  in a given line below have the same value modulo-6.

$$\begin{aligned} \dots &= (-9)_6 = (-3)_6 = \underline{(3)}_6 = (9)_6 = (15)_6 = \dots = 3 \text{ mod } 6 \\ \dots &= (-8)_6 = \underline{(-2)}_6 = (4)_6 = (10)_6 = \dots = -2 \text{ mod } 6 \\ \dots &= (-7)_6 = \underline{(-1)}_6 = (5)_6 = (11)_6 = \dots = -1 \text{ mod } 6 \\ \dots &= (-6)_6 = \underline{(0)}_6 = (6)_6 = (12)_6 = \dots = 0 \text{ mod } 6 \\ \dots &= (-5)_6 = \underline{(1)}_6 = (7)_6 = (13)_6 = \dots = 1 \text{ mod } 6 \\ \dots &= (-4)_6 = \underline{(2)}_6 = (8)_6 = (14)_6 = \dots = 2 \text{ mod } 6 \\ \dots &= (-3)_6 = \underline{(3)}_6 = (9)_6 = (15)_6 = \dots = 3 \text{ mod } 6 \\ \dots &= (-8)_6 = \underline{(-2)}_6 = (4)_6 = (10)_6 = \dots = -2 \text{ mod } 6 \end{aligned} \quad (7.3.7)$$

How do we choose a  $k_m$  number label? We choose the underlined ones with the smallest  $|m|$  and pick the positive one if two are equal. This choice  $\{m=-2, -1, 0, 1, 2, 3\}$  of  $N=6$   $m$ -values is used in Fig. 7.3.2.

### (b) Discrete orthonormality and completeness

Orthonormality relations for wave states reduce to finite geometric sums.

$$\langle k_m' | k_m \rangle = \sum_{p=0}^{N-1} \frac{e^{-ik' m' x_p}}{\sqrt{N}} \frac{e^{ik m x_p}}{\sqrt{N}} = \frac{1}{N} \sum_{p=0}^{N-1} e^{i(k m - k' m') x_p}, \text{ where: } x_p = p a \quad (7.3.8a)$$

Substituting (7.3.2) and (7.3.5) gives

$$\langle k_m' | k_m \rangle = \sum_{p=0}^{N-1} z^p = \frac{1+z+z^2+\dots+z^{N-1}}{N}, \text{ where: } z = e^{i(k m - k' m') a} = e^{i2\pi(m-m')/N}$$

The geometric sum yields a result that satisfies  $k_m$ -orthonormality axiom-3.

$$\langle k_m' | k_m \rangle = \frac{1}{N} \frac{1-z^N}{1-z} = \frac{1}{N} \frac{1-e^{i2\pi(m-m')}}{1-e^{i2\pi(m-m')/N}} = \delta_{mm'} \quad (7.3.8b)$$

The  $k_m$ -completeness axiom-4 (or  $x_p$ - orthonormality) is satisfied for these wave states, as well.

$$\langle x_p' | x_p \rangle = \sum_{m=0}^{N-1} \langle x_p' | k_m \rangle \langle k_m | x_p \rangle = \sum_{m=0}^{N-1} \frac{e^{ik m x_p'}}{\sqrt{N}} \frac{e^{-ik m x_p}}{\sqrt{N}} = \frac{1}{N} \sum_{m=0}^{N-1} e^{i(x_p' - x_p) k m} = \delta_{pp'} \quad (7.3.9)$$

**(c) Discrete Fourier transformation matrices**

Below are shown Fourier transformation matrices and discrete  $x_p$ -wavefunctions (7.3.5b)

$$\langle k_m | x_p \rangle = \Psi_{k_m}(x_p)^* = e^{-ik_m x_p} / \sqrt{N} \tag{7.3.10a}$$

They are drawn as complex phasor amplitudes for the cyclic  $N$ -state systems ( $C_N$ ) for  $N= 1, 2, 3, 4, 5,$  and  $6$ .

Also drawn over the phasors is the Re-part of the "Bohr's ghost" continuum  $x$ -wavefunctions

$$\langle k_m | x \rangle = \Psi_{k_m}(x)^* = e^{-ik_m x} / \sqrt{L} \tag{7.3.10b}$$

Recall (7.1.10) or Fig. 7.1.1. "Bohr's ghosts" match the discrete waves (7.3.10a) with phasor clocks.

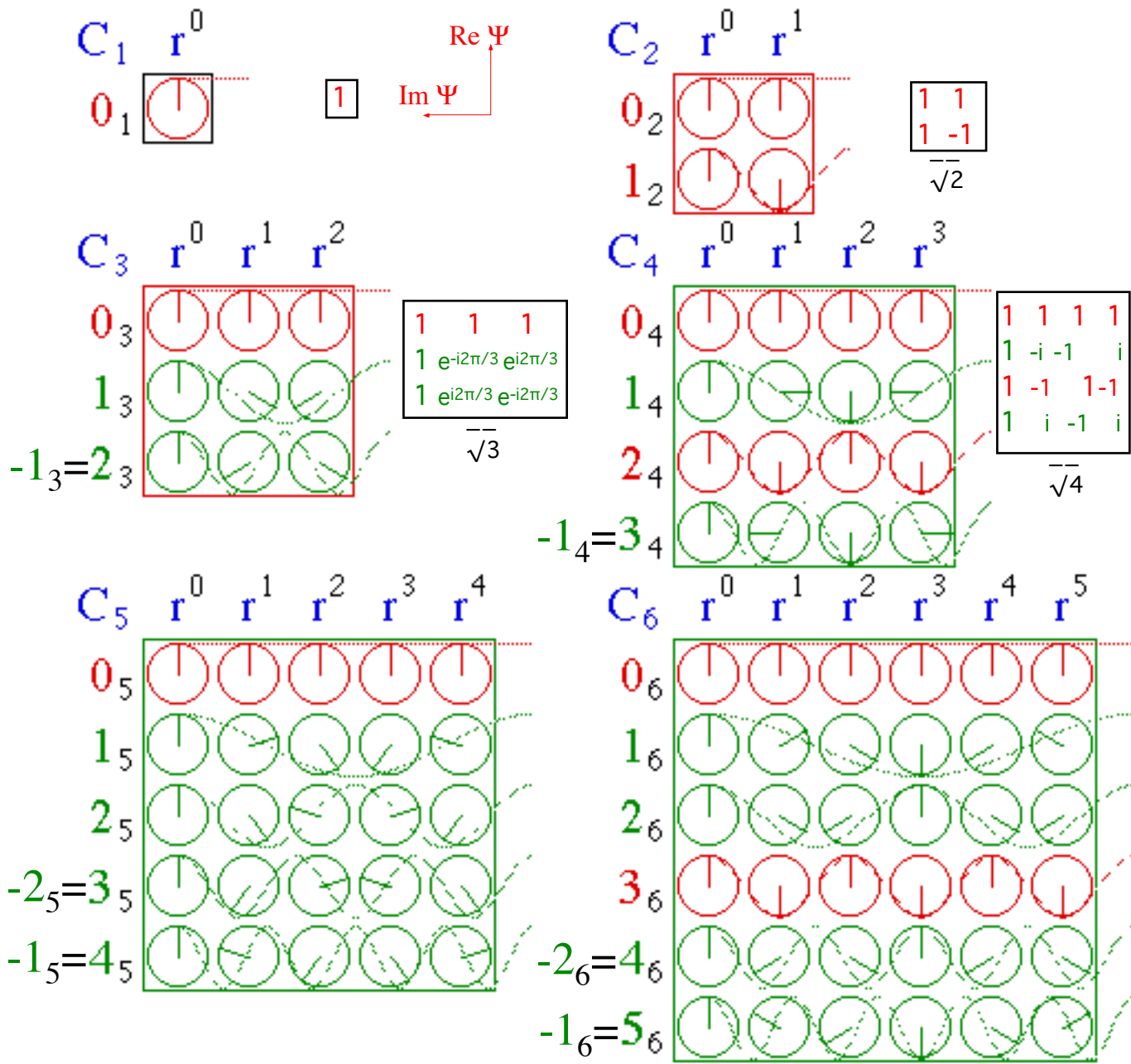


Fig.

7.3.3 Discrete Fourier transformation matrices for  $N$ -cyclic ( $C_N$ ) systems ( $N = 1, 2, \dots, 6\dots$ )

### (d) Introducing aliases and Brillouin zones

It is important to see the relation between the continuum waves and their "course-grained" images thatves with integral wave-numbers of  $m \bmod N$  whole wavelengths within each  $\langle k_m |$ -row of phasors. We might as well call them "row-waves" or "bra-waves." Note also, that the same wave shape exists in the columns or kets  $|x_p\rangle$ . Each "ket-wave"  $|x_p\rangle$  represents a  $\delta$ -position state or "pulse" localized at point  $x_p$ . The inverse Fourier transformation  $\langle k_m |x_p\rangle$  relates  $|x_p\rangle$  to a bra-wave  $\langle k_m |$ . As required by conjugation axiom-2, namely,  $\langle k_m |x_p\rangle = \langle x_p |k_m\rangle^*$ , the relation is the same as between  $|k_m\rangle$  and  $\langle x_p |$ , except for conjugation.

For low wave number like, say  $(m_N)=(1)_6$  or  $(2)_6$ , it is easy to see the "Bohr's-ghost wave" mirrored in the phasors as in the second and third row of the  $C_6$  matrix in Fig. 7.3.1. Note however, that these phasors are set so the phase of the one to the right is clockwise (that is it appears ahead) of the one to the left. This means, if the phasors turned clockwise, that the one to the right is feeding energy into the one to its left, so the wave would be moving right-to-left with wave momentum minus  $(1)_6$  or minus  $(2)_6$ , respectively. But, they're conjugated bras so their clocks go backwards and so the labels are OK, after all.

For high wave number like, say  $(m_N)=(4)_6$  or  $(5)_6$ , it is not so easy to see the "Bohr's-ghost wave" mirrored in the phasors as in the fifth and sixth row of the  $C_6$  matrix in Fig. 7.3.1. But, you can see *alias* waves of negative wave momentum  $(m_N)=(-2)_6$  or  $(-1)_6$ , respectively, that is oppositely moving waves of low wavenumber. Recall that  $(4 \bmod 6)$  equals  $(-2 \bmod 6)$  and  $(5 \bmod 6)$  equals  $(-1 \bmod 6)$ .

Right in the middle row of the *even-N* matrix is a wave that isn't going in either direction. In the  $C_6$  matrix it is the  $(3)_6$  wave. Since  $(3 \bmod 6)$  equals  $(-3 \bmod 6)$  this is a good old push-me-pull-you standing wave with all real amplitudes of  $(1, -1, 1, -1, 1, -1)$ . This can only happen for even- $N$  and is known as a *first Brillouin zone boundary* wave in solid-state physics.

All cases have a zero-momentum wave  $(0_N)$  at the top of the transformation matrix. This is called the *Brillouin zone center* wave in solid-state physics. Indeed, it is centered at the bottom of the dispersion plot in Fig. 2.6.1. Its phasor settings are the same as that of a higher  $(N_N)$ , or  $(2N_N)$ , or  $(3N_N)$ , ...etc. wave. However, this  $N$ -state system does not count higher than  $N-1$  without recycling.

Consider, for example, a  $k_{-11}$  wave of wavevector  $(-11)_{12}$  (with minus-eleven-kinks-modulo-12) as plotted in Fig. 7.3.4 (a). Since  $(-11)\text{-mod-}12$  equals  $(+1)\text{-mod-}12$  (that is,  $(-11)_{12}=(+1)_{12}$ ) it follows that the wave shown has the same effect as a  $(+1)_{12}$  wave. Indeed, the twelve masses in Fig. 7.3.4(a) line up on a single-kink ( $k=1$ )-wave moving positively, while the ( $k=-11$ )-wave moves negatively. (See *WaveIt* movie.) This is an example of aliasing. In a  $C_{12}$  lattice,  $(k=-11)$  is an alias for  $(k=+1)$ .

Fig. 7.3.4(b) shows the  $k$ -space with a typical frequency dispersion function plotted above it. The difference between any two alias wavevectors such as  $(k=+1)$  and  $(k=-11)$  is a *reciprocal lattice vector*  $k_{12}$  or  $(12)_{12}=(0)_{12}$ . The reciprocal lattice vector  $k_{12}$  also spans the first Brillouin-zone from  $(-6)_{12}$  to  $(+6)_{12}$  as shown at the bottom of the figure. An important idea here is that a wavevector  $k$ -space must have the same  $N$ -fold periodic symmetry as the coordinate  $x$ -space. Moving across row of a  $\langle k_m |x_p\rangle$  matrix gives the same variation as moving up the corresponding column since  $\langle k_m |x_p\rangle$  is unitary. Both are  $N$ -fold periodic!

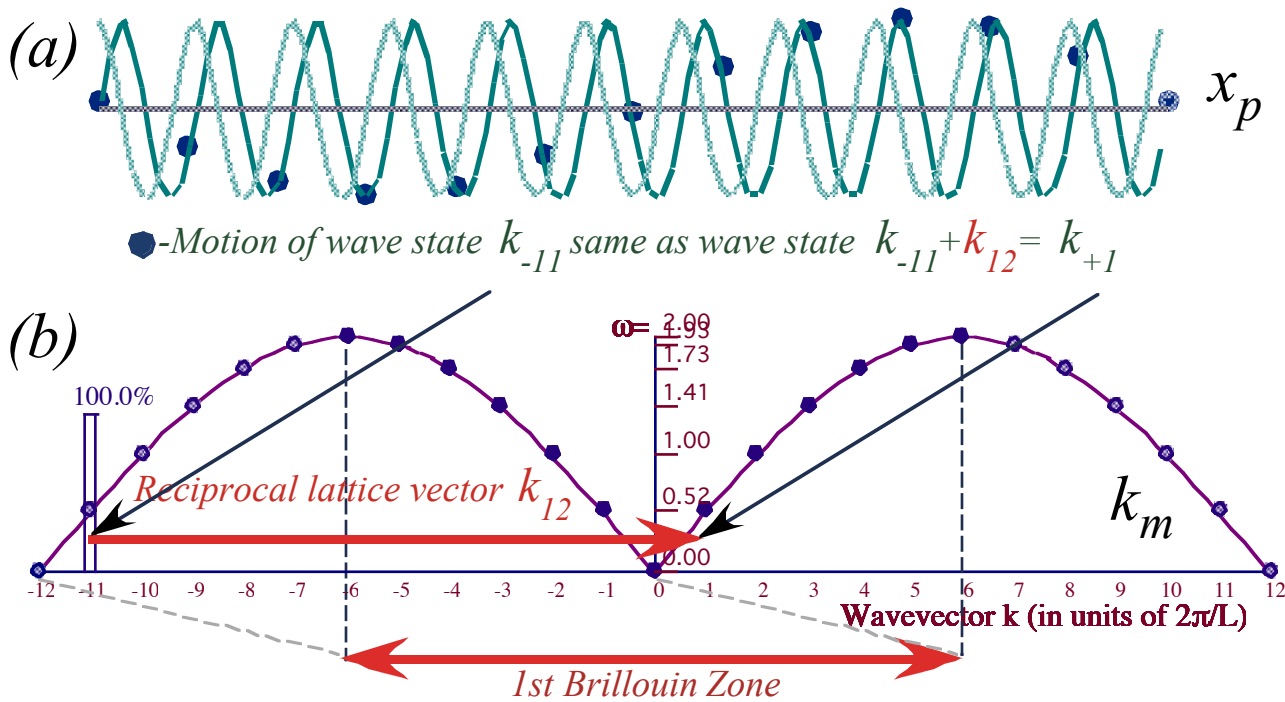


Fig. 7.3.4 (a) (-11)-wave has the same effect as its alias (+1)-wave. (b) Difference is zone vector  $k_{12}$ .

To appreciate the symmetry of a Fourier transform matrix, it may help to examine some larger ones. For example, Fig. 7.3.5 shows the Fourier matrix for  $N=24$ . Phase of each amplitude  $\langle k_m | x_p \rangle$  is color coded so it can be more easily spotted. Symmetry patterns should now be more evident. Remember, that these patterns repeat forever in all directions right and left or up and down in a great checkerboard quilt!

This beginning discussion of discrete wave analysis should make it clear that there is considerable physical and mathematical complexity hiding in these "simple" Fourier structures. Indeed, this is a key to understanding fundamental quantum symmetry properties and techniques which are generally labeled by a mathematical misnomer as "group theory." We shall explore some more of this shortly.

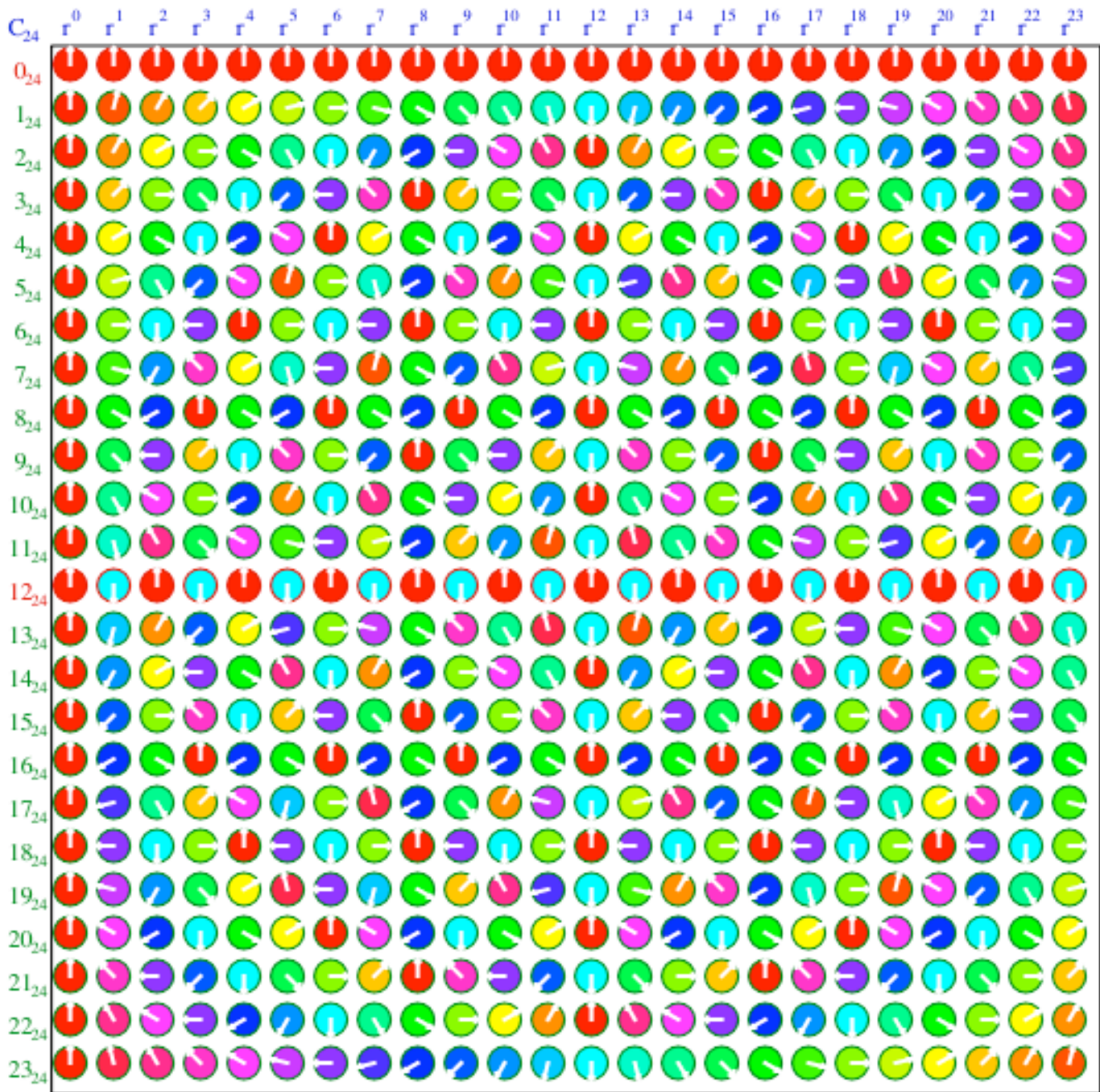


Fig. 7.3.5 Phase color coded Fourier transformation matrix for  $N=24$ .



## Problems for Chapter 7

### Bohring problems

**7.1.1.** For a Bohr ring of fixed circumference  $L = 1nm$  consider the following wavefunction  $\Psi(x) = \langle x | \Psi \rangle$  distributions around the ring at  $t=0$ , and deduce the amplitudes  $\langle m | \Psi \rangle$  of each of the eigenstates  $|m\rangle$  for  $m=0, \pm 1, \pm 2, \dots$ . Let the eigenfrequencies be  $\nu_m = (0, 1, 4, \dots, m^2, \dots)MHz$ .

(a)  $\Psi(x) = \text{const.}$  .

(b)  $\Psi(x) = \text{const.}(1 + \cos 2\pi x/L)$  .

(c)  $\Psi(x) = \text{const.}$  for  $-L/4 < x < L/4$  and  $\Psi(x) = 0$  elsewhere.

For each case evaluate *const.* assuming one particle occupies the ring.

(d) For each case (a) to (c) answer: "Is it a stationary state?" If not, calculate, plot, and discuss the wavefunctions of each case at time  $t = 1\mu\text{sec}$ , and at  $0.5\mu\text{sec}$  .

### Continuously boring problems

**7.2.1.** For an infinite line ( $-\infty < x < \infty$ ) consider the following wavefunction  $\Psi(x) = \langle x | \Psi \rangle$  distributions along the line. Calculate, plot, and discuss the amplitude functions  $\langle k | \Psi \rangle$  of each of the eigenstates  $|k\rangle$  for ( $-\infty < k < \infty$ ). Let the eates  $|k\rangle$  for ( $-\infty < k < \infty$ ). Let the eigenfrequencies be  $\nu_k = (kL/2\pi)^2 MHz$ . (Let unit length be  $L = 1nm$ .)

(a)  $\Psi(x) = \text{const.}$  .

(b)  $\Psi(x) = \text{const.}(1 + \cos 2\pi x/L)$  . .

(c)  $\Psi(x) = \text{const.}$  for  $-L/4 < x < L/4$  and  $\Psi(x) = 0$  elsewhere.

Evalu per unit length ( $L = 1nm$ ).

(d) For each case (a) to (c) answer: "Is it a stationary state?" If not, calculate, plot, and discuss the wavefunctions of each case at time  $t = 1\mu\text{sec}$ , and at  $0.5\mu\text{sec}$  .

### Continuously discrete or discretely continuous?

**7.3.1.** Ch.7 contains discussion of 1D Fourier wave systems with (a) Continuous  $x$  and discrete  $k$ , (b) Continuous  $x$  and continuous  $k$ , and (c) Discrete  $x$  and discrete  $k$ . Using physical models of each to discuss how physically relizeable these are. Is there a 4th possibility? Discuss.

### Aliases on the move

**7.3.2.** Consider the two aliases (-1) and (+1) in Fig. 7.3.4. Discuss whether a dispersion function  $\omega(k)$  should repeat periodically. Should the period be the zone vector  $k_{12}$ ? For computation use  $\omega(k) = |\sin(\pi k/12)|$  as plotted where  $k=0, \pm 1, \pm 2, \pm 3, \dots$  in units of  $2\pi/L$ . Use  $V_{\text{phase}} = \omega/k$  and  $V_{\text{group}} = d\omega/dk$  .

(a) Is the phase velocity the same for the two alias states (-1) and (+1)? Compute and discuss why or why not.

(a) Is the group velocity the same for the two alias states (-1) and (+1)? Compute and discuss why or why not.