Topics in mathematical physics

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CONTENTS

I. FOURIER ANALYSIS

We will first study Fourier series of periodic functions, then study Fourier transform for general functions. These two topics are related, and we will call them together as Fourier analysis. They are widely used in, among other things, all kinds of wave phenomena and the physics of solids (which has a periodic crystalline environment).

A. Fourier series

1. General properties

First, recall that the periods of $\sin \alpha x$ and $\cos \alpha x$ are $\frac{2\pi}{\alpha}$. Hence, the periods of $\sin \frac{2\pi}{a}nx$ and $\cos \frac{2\pi}{a}nx$ ($n = 1, 2, 3\cdots$) are $\frac{a}{n}$. It is obvious that

$$\int_0^a dx \sin \frac{2\pi}{a}nx = 0, \tag{1.1}$$

$$\text{and} \int_0^a dx \cos \frac{2\pi}{a}nx = 0. \tag{1.2}$$

The interval of integration can be shifted to $[-a/2+\delta, a/2+\delta]$ ((δ is arbitrary) without changing the results. Furthermore, it can be shown that

$$\int_0^a dx \sin \frac{2\pi}{a}mx \sin \frac{2\pi}{a}nx = \frac{a}{2}\delta_{mn}, \tag{1.3}$$

$$\int_0^a dx \sin \frac{2\pi}{a}mx \cos \frac{2\pi}{a}nx = 0, \tag{1.4}$$

$$\int_0^a dx \cos \frac{2\pi}{a}mx \cos \frac{2\pi}{a}nx = \frac{a}{2}\delta_{mn}. \tag{1.5}$$

Again the interval of integration can be shifted at will, e.g., to $[-a/2, a/2]$. This practice applies to all of the periodic integrands integrated over a period below. These three equations are called **orthogonality relations**. You need to memorize them, since they are *really* useful.

Fourier theorem:
Suppose $f(x)$ is a periodic function with period a, and $|f(x)|^2$ is integrable over the interval $[0, a]$, then $f(x)$ can be expanded by $\sin \frac{2\pi}{a}nx$ and $\cos \frac{2\pi}{a}nx$,

$$f(x) = a_0 + \sum_{n=1}^{\infty}\left(a_n \cos \frac{2\pi}{a}nx + b_n \sin \frac{2\pi}{a}nx\right). \tag{1.6}$$

First, it is easy to check that $f(x+a) = f(x)$. Next, we can use the orthogonality relations to find out the coefficients $\{a_0, a_n, b_n; n \geq 1\}$,

$$a_0 = \frac{1}{a}\int_0^a dx f(x) \equiv \langle f\rangle_a, \tag{1.7}$$

$$a_n = \frac{2}{a}\int_0^a dx f(x) \cos \frac{2\pi}{a}nx, \tag{1.8}$$

$$b_n = \frac{2}{a}\int_0^a dx f(x) \sin \frac{2\pi}{a}nx. \tag{1.9}$$

Note that a_0 is simply the average of $f(x)$ over a period a. The necessity of $f(x)$ being square integrable over a period will be explained later.

We can use Dirac's bracket notation and define

$$\langle f|g\rangle = \int_0^a dx f^*(x) g(x). \tag{1.10}$$

This is called the **inner product** of f and g. Furthermore, write $\cos \frac{2\pi}{a}nx$ and $\sin \frac{2\pi}{a}nx$ simply as $\hat{c}_n$ and $\hat{s}_n$.

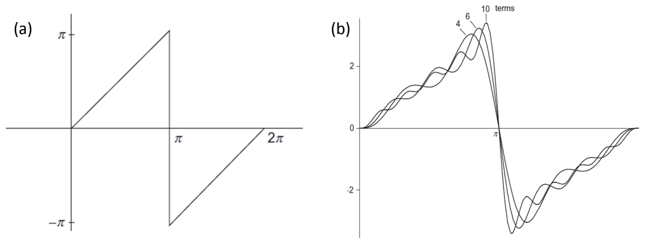

FIG. 1 (a) An unit of a sawtooth wave. (b) The superposition of many sinusoidal waves from a Fourier series.

Then the Fourier series is,

$$f = a_0 + \sum_{n=1}^{\infty} \left(a_n \hat{c}_n + b_n \hat{s}_n \right). \tag{1.11}$$

The orthogonality relations are,

$$\langle \hat{s}_m | \hat{s}_n \rangle = \frac{a}{2} \delta_{mn}, \tag{1.12}$$

$$\langle \hat{s}_m | \hat{c}_n \rangle = 0, \tag{1.13}$$

$$\langle \hat{c}_m | \hat{c}_n \rangle = \frac{a}{2} \delta_{mn}. \tag{1.14}$$

The coefficients are,

$$a_0 = \frac{1}{a} \langle 1 | f \rangle, \tag{1.15}$$

$$a_n = \frac{2}{a} \langle \hat{c}_n | f \rangle, \tag{1.16}$$

$$b_n = \frac{2}{a} \langle \hat{s}_n | f \rangle. \tag{1.17}$$

These shorthand notations reveal clearly the overall "structure" of the Fourier series.

2. Parity symmetry

If $h(x)$ is an *odd* function with respect to the origin, $h(-x) = -h(x)$, then

$$\int_{-L}^{L} dx h(x) = \int_{-L}^{0} dx h(x) + \int_{0}^{L} dx h(x) \tag{1.18}$$

$$= \int_{L}^{0} dx' h(x') + \int_{0}^{L} dx h(x), \ (x' \equiv -x)$$

$$= 0. \tag{1.19}$$

The area below the curve $h(x)$ for $x < 0$ cancels with the one for $x > 0$.

With this property, we show that if $f(x)$ has parity symmetry with respect to the origin, then the loading of the calculation can be halved. That is:
1. If $f(x)$ is an even function, $f(-x) = f(x)$, then $b_n = 0$ for any n;
2. If $f(x)$ is an odd function, $f(-x) = -f(x)$, then $a_n = 0$ for any n.

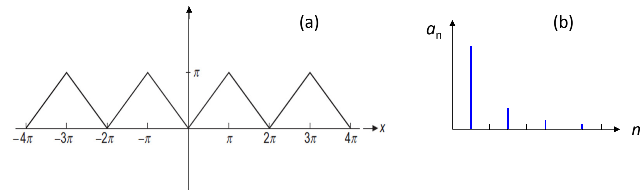

FIG. 2 (a) A triangular wave. (b) The spectral analysis of the triangular wave.

For example, if $f(x)$ is an even function, then

$$b_n = \frac{2}{a} \int_{-a/2}^{a/2} dx f(x) \sin \frac{2\pi}{a} nx \tag{1.20}$$

$$= 0 \tag{1.21}$$

The integral is zero because the integrand $h(x) \equiv f(x) \sin \frac{2\pi}{a} nx$ is an odd function, $h(-x) = -h(x)$. Similar proof applies to the case when $f(x)$ is an odd function.
Ex 1: Find the Fourier series expansion of the sawtooth wave,

$$f(x) = \begin{cases} x, & 0 \le x < \pi, \\ x - 2\pi, & \pi < x \le 2\pi. \end{cases} \tag{1.22}$$

Sol'n: The function $f(x)$ is shown in Fig. 1(a). It is convenient to write it as

$$f(x) = x, \quad x \in [-\pi, \pi], \text{ period } a = 2\pi. \tag{1.23}$$

Since $f(x)$ is an odd function, all of the coefficients a_n (including a_0) would vanish. It is not difficult to find out that,

$$b_n = \frac{2}{2\pi} \int_{-\pi}^{\pi} dx x \sin nx \tag{1.24}$$

$$= 2 \frac{(-1)^n}{n} \sim \frac{1}{n}. \tag{1.25}$$

Thus,

$$f(x) = 2 \left(\sin x - \frac{\sin 2x}{2} + \frac{\sin 3x}{3} + \cdots \right). \tag{1.26}$$

With more terms, the sum from the RHS would approach the sawtooth wave on the LHS, see Fig. 1(b). If $x = \pi/2$, then one has

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots. \tag{1.27}$$

This is **Leibniz's formula**.
Ex 2: Find the Fourier series expansion of the triangular wave (Fig. 2(a)),

$$f(x) = \begin{cases} +x, & 0 < x \le \pi, \\ -x, & -\pi < x \le 0. \end{cases} \tag{1.28}$$

$$\text{or} = |x|, x \in [-\pi, \pi], \ a = 2\pi. \tag{1.29}$$

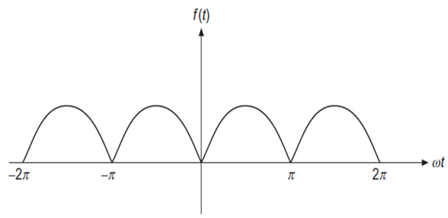

FIG. 3 The wave produced by a full-wave rectifier.

Sol'n: This is an even function so we only have to calculate a_n. First,

$$a_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx|x| \quad (1.30)$$
$$= \frac{\pi}{2}. \quad (1.31)$$

Second,

$$a_n = \frac{2}{2\pi}\int_{-\pi}^{\pi} dx|x|\cos nx \quad (1.32)$$
$$= -\frac{4}{\pi}\frac{1}{n^2}, \quad n \in \text{odd integer}. \quad (1.33)$$

The distribution of a_n is shown in Fig. 2(b). Thus,

$$f(x) = \frac{\pi}{2} - \frac{4}{\pi}\sum_{n\,\in\,\text{odd}}^{\infty}\frac{\cos nx}{n^2}. \quad (1.34)$$

Let $x = \pi$, then we will have

$$\frac{\pi^2}{8} = 1 + \frac{1}{3^2} + \frac{1}{5^2} + \cdots \quad (1.35)$$

This series converges faster than the one in Eq. (1.27).

If we differentiate both sides of Eq. (1.34), then

$$f'(x) = \frac{4}{\pi}\sum_{n\,\in\,\text{odd}}\frac{\sin nx}{n}. \quad (1.36)$$

This would be the Fourier series expansion of a square wave. It converges slowly ($\sim 1/n$) compared to the triangular wave ($\sim 1/n^2$). This is a general feature of the Fourier series: The smoother the function, the faster the convergence of its Fourier series.

Ex 3: Find the Fourier series expansion of the rectified wave in Fig. 3,

$$f(t) = \begin{cases} +\sin\omega t, & 0 < \omega t \le \pi, \\ -\sin\omega t, & -\pi < \omega t \le 0. \end{cases} \quad (1.37)$$

Sol'n: This is an even function so we only have to calculate a_n. First,

$$a_0 = \frac{1}{\pi}\int_0^{\pi} d\omega t \sin\omega t \quad (1.38)$$
$$= \frac{2}{\pi}. \quad (1.39)$$

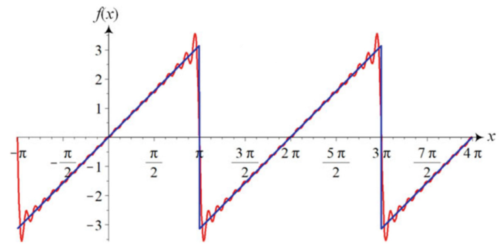

FIG. 4 The Fourier series overshoots the sawtooth wave at discontinuities.

Second,

$$a_n = \frac{2}{\pi}\int_0^{\pi} d\omega t \sin\omega t\cos n\omega t \quad (1.40)$$
$$= \begin{cases} 0, & n \in \text{odd} \\ -\frac{2}{\pi}\frac{2}{n^2-1}, & n \in \text{even}. \end{cases} \quad (1.41)$$

Thus,

$$f(t) = \frac{2}{\pi} - \frac{4}{\pi}\left(\frac{\cos 2\omega t}{2^2-1} + \frac{\cos 4\omega t}{4^2-1} + \cdots\right). \quad (1.42)$$

More examples of the Fourier series can be found in, e.g., https://www.falstad.com/fourier/e-index.html.

Finally, we comment on a peculiar feature of the Fourier series. If $f(x)$ is *discontinuous*, as the sawtooth wave in Example 1, then near a discontinuity, the sum of the series would "overshoot" by about 18 % (Fig. 4). This is called **Gibbs phenomena**. This overshoot cannot be removed by summing more terms in the Fourier series. Also, at a point x_0 of discontinuity, the Fourier series converges to

$$\lim_{\varepsilon\to 0}\frac{1}{2}\left[f(x_0+\varepsilon) + f(x_0-\varepsilon)\right]. \quad (1.43)$$

3. Exponential bases

Instead of expanding with $\sin x$ and $\cos x$, one can expand the Fourier series with e^{ix}. First, write

$$\cos\frac{2\pi}{a}nx = \frac{1}{2}\left(e^{i\frac{2\pi}{a}nx} + e^{-i\frac{2\pi}{a}nx}\right), \quad (1.44)$$
$$\sin\frac{2\pi}{a}nx = \frac{1}{2i}\left(e^{i\frac{2\pi}{a}nx} - e^{-i\frac{2\pi}{a}nx}\right), \quad (1.45)$$

then

$$f(x) = a_0 + \sum_{n=1}^{\infty}\left(a_n\cos\frac{2\pi}{a}nx + b_n\sin\frac{2\pi}{a}nx\right)$$
$$= \sum_{n=-\infty}^{\infty} c_n e^{i\frac{2\pi}{a}nx}, \quad (1.46)$$

in which $(n > 0)$

$$c_0 = a_0, \tag{1.47}$$

$$c_n = \frac{1}{2}(a_n - ib_n), \tag{1.48}$$

$$c_{-n} = \frac{1}{2}(a_n + ib_n) = c_n^*. \tag{1.49}$$

There is only one orthogonality relation,

$$\int_0^a dx e^{-i\frac{2\pi}{a}nx} e^{i\frac{2\pi}{a}mx} = a\delta_{mn}. \tag{1.50}$$

Using this relation, one can find the coefficients of expansion,

$$c_n = \frac{1}{a}\int_0^a dx f(x) e^{-i\frac{2\pi}{a}nx}. \tag{1.51}$$

With the shorthand notation $\hat{e}_n \equiv e^{i\frac{2\pi}{a}nx}$, the Fourier series becomes,

$$f = \sum_n c_n \hat{e}_n. \tag{1.52}$$

The orthogonality relation is

$$\langle \hat{e}_n | \hat{e}_m \rangle = a\delta_{mn}, \tag{1.53}$$

from which we get the coefficients of expansion,

$$c_n = \frac{1}{a}\langle \hat{e}_n | f \rangle. \tag{1.54}$$

Some general properties of the Fourier series are listed below:

Property 1. If

$$\sum_{n=-\infty}^{\infty} c_n e^{i\frac{2\pi}{a}nx} = 0, \tag{1.55}$$

then $c_n = 0$ for any n. This can be easily proved by identifying the 0 on the RHS with $f(x)$ and applying Eq. (1.51).

Property 2. If

$$\sum_{n=-\infty}^{\infty} c_n e^{i\frac{2\pi}{a}nx} = \sum_{n=-\infty}^{\infty} d_n e^{i\frac{2\pi}{a}nx}, \tag{1.56}$$

then $c_n = d_n$ for any n. This can be proved by moving two summations to the same side of the equation and identifying $c_n - d_n$ with the c_n in Property 1.

Property 2 shows that the Fourier series expansion of a function $f(x)$ must be unique. There cannot be two different expansions that sum up to the same function $f(x)$.

3. The inner product between two functions is

$$\langle f | g \rangle = \sum_{nm} c_n^* d_m \langle \hat{e}_n | \hat{e}_m \rangle \tag{1.57}$$

$$= a \sum_n c_n^* d_n. \tag{1.58}$$

Hence,

$$\langle f | f \rangle = a \sum_n |c_n|^2. \tag{1.59}$$

These properties seem to be familiar because they are analogous to the expansion of a vector,

$$\mathbf{v} = v_1 \hat{\mathbf{e}}_1 + v_2 \hat{\mathbf{e}}_2 + v_3 \hat{\mathbf{e}}_3. \tag{1.60}$$

If the bases are orthogonal,

$$\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \delta_{ij} \tag{1.61}$$

then the coefficients of expansion are uniquely determined, and

$$v_i = \hat{\mathbf{e}}_i \cdot \mathbf{v}. \tag{1.62}$$

Also, the inner product between two vectors are,

$$\mathbf{u} \cdot \mathbf{v} = \sum_i u_i v_i. \tag{1.63}$$

Here $\{\hat{e}_n\}$ plays the role of the orthogonal bases $\{\hat{e}_i\}$, and c_n plays the role of the coefficient of expansion v_i. However, note that

1. The dimension of the "vector space" for $f(x)$ is infinite.
2. The components of the $f(x)$-vector can be complex-valued.

Such a vector space for functions is called a **Hilbert space**. One requirement for the functions $f(x)$ in the Hilbert space is that they have to be **square integrable**. That is, their "length", $|f| = \sqrt{\langle f | f \rangle}$, has to be finite.

In quantum mechanics, a wave function $\psi(x)$ is such a *state vector* in Hilbert space. According Born's interpretation, $|\psi(x)|^2 dx$ is the probability of finding the particle within the interval dx, and

$$\int_{-\infty}^{\infty} dx |\psi(x)|^2 = 1. \tag{1.64}$$

Therefore, $\psi(x)$ needs to be normalizable (or square integrable) to fit in such a theoretical framework.

B. Fourier transform

In general, an integral transform of a function $f(t)$ has the following form,

$$f(t) \to g(s) = \int_b^a dt f(t) K(s,t), \tag{1.65}$$

in which $K(s,t)$ is called a **kernel** of the integral transform. For example, Fourier transform is given as

$$g(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{i\omega t}. \tag{1.66}$$

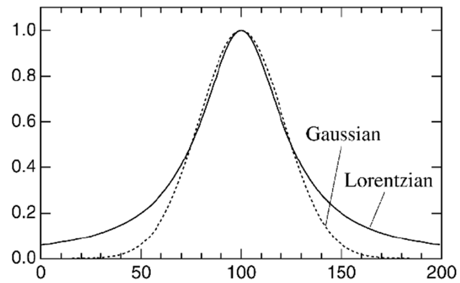

FIG. 5 Lorentzian distribution vs Gaussian distribution.

and Laplace transform is

$$g(s) = \int_0^\infty dt f(t) e^{-st}. \tag{1.67}$$

We will discuss only the Fourier transform in this Note.

Write an integral transform as

$$f(t) \to g(s) = \mathcal{L}f(t) \equiv \int_b^a dt f(t) K(s,t). \tag{1.68}$$

It is then clear that

$$\mathcal{L}(cf) \;=\; c\mathcal{L}f, \; c \text{ is a const} \tag{1.69}$$
$$\mathcal{L}(f_1 + f_2) \;=\; \mathcal{L}f_1 + \mathcal{L}f_2. \tag{1.70}$$

That is, an integral transform is a linear transformation.

In physics, if $f(t)$ is a function of time t, then the kernel of the Fourier integral, $K(\omega, t) = e^{i\omega t}$, is a harmonic oscillation with frequency ω. The Fourier integral can be considered as a superposition of these oscillations that sums up to $f(t)$.

Fourier transform can help us solving linear differential equations. For example, the *differential equation* for $f(t)$ would become an *algebraic equation* for $g(\omega)$. After solving for $g(\omega)$, one can then obtain $f(t)$ by performing an inverse Fourier transform on $g(\omega)$:

$$\begin{array}{ccc} \text{Diff eq for } f(t) & \xrightarrow{transform} & \text{Alg eq for } g(\omega) \\ & & \downarrow \text{solve} \\ f(t) & \xleftarrow{inverse\ tranf} & g(\omega) \end{array} \tag{1.71}$$

We will learn how to do this in this Note.

1. Fourier integral

Ex 1: Given $f(t) = e^{-\alpha|t|}$ ($\alpha > 0$), one has

$$g(\omega) \;=\; \int_{-\infty}^{\infty} dt e^{-\alpha|t|} e^{i\omega t} \tag{1.72}$$
$$=\; \frac{2\alpha}{\omega^2 + \alpha^2}, \tag{1.73}$$

which is a **Lorentzian distribution** (Fig. 5). Its half-width is roughly of the order of α.

Ex 2: Consider the **Gaussian distribution**, $f(t) = e^{-\alpha t^2}$ ($\alpha > 0$). Its half-width is roughly of the order of $1/\sqrt{\alpha}$ (Fig. 5). Its Fourier transform,

$$g(\omega) \;=\; \int_{-\infty}^{\infty} dt e^{-\alpha t^2} e^{i\omega t} \tag{1.74}$$
$$=\; \sqrt{\frac{\pi}{\alpha}} e^{-\omega^2/4\alpha}, \tag{1.75}$$

which is also a Gaussian distribution. Its half-width is roughly of the order of $\sqrt{\alpha}$. It can be seen that if α gets smaller, then $f(t)$ gets broader, but $g(\omega)$ gets sharper (Fig. 6).

2. Dirac delta function

Before introducing the inverse Fourier transform, let's have a brief review of the Dirac delta function. The Dirac delta function is an *even* function that satisfies the following properties,

$$1. \quad \delta(x - x_0) = \begin{cases} \infty & x = x_0 \\ 0 & x \neq x_0 \end{cases} \tag{1.76}$$
$$2. \quad \int_{-\infty}^{\infty} dx \delta(x - x_0) = 1, \tag{1.77}$$
$$3. \quad \int_{-\infty}^{\infty} dx f(x) \delta(x - x_0) = f(x_0). \tag{1.78}$$

The second property shows that the "area" below the delta function distribution is one. Among other properties of the delta function, here we cite only one (c is a constant)

$$\delta[c(x - x_0)] = \frac{1}{|c|} \delta(x - x_0). \tag{1.79}$$

Ex 3: Given a **Dirac delta function**, $f(t) = \delta(t - t_0)$, one has

$$g(\omega) \;=\; \int_{-\infty}^{\infty} dt \delta(t - t_0) e^{i\omega t} \tag{1.80}$$
$$=\; e^{i\omega t_0}. \tag{1.81}$$

Note that $f(t)$ is infinitely sharp, while its Fourier transform $|g(\omega)| = 1$ is flat.

The Dirac delta function can be considered as the limit of a very sharp distribution. There are different choices of such distributions, as long as they can satisfy the requirements above. For example, both the Lorentzian distribution and the Gaussian distribution above could approach the delta function when $\alpha \to 0$. Write

$$g_\alpha^L(x) \;=\; \frac{2\alpha}{x^2 + \alpha^2}, \tag{1.82}$$
$$g_\alpha^G(x) \;=\; e^{-x^2/4\alpha}, \tag{1.83}$$

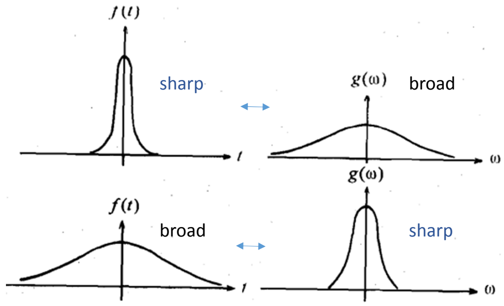

FIG. 6 A Gaussian curve and its Fourier transformation. When one is narrow, the other is broad.

then the areas below this two curves are

$$\int_{-\infty}^{\infty} dx g_\alpha^L(x) = 2\tan^{-1}\frac{x}{\alpha}\Big|_{-\infty}^{\infty} = 2\pi, \quad (1.84)$$
$$\int_{-\infty}^{\infty} dx g_\alpha^L(x) = 2\pi. \quad (1.85)$$

Thus, define

$$\delta_\alpha(x) = \frac{1}{2\pi}g_\alpha^L(x) = \frac{\alpha/\pi}{x^2+\alpha^2}, \quad (1.86)$$
$$\text{or } \delta_\alpha(x) = \frac{1}{2\pi}g_\alpha^G(x) = \frac{1}{\sqrt{4\pi\alpha}}e^{-x^2/4\alpha}. \quad (1.87)$$

Both would lead to

$$\lim_{\alpha\to 0}\delta_\alpha(x-x_0) = \delta(x-x_0), \quad (1.88)$$

From Example 1, we get

$$\int_{-\infty}^{\infty} dt e^{-\alpha|t|}e^{i\omega t} = 2\pi\delta_\alpha(\omega), \quad (1.89)$$
$$\text{let } \alpha\to 0, \text{ then } \int_{-\infty}^{\infty} dt e^{i\omega t} = 2\pi\delta(\omega). \quad (1.90)$$

The second equation can be written in alternative forms,

$$\int_{-\infty}^{\infty} dt e^{i(\omega-\omega_0)t} = 2\pi\delta(\omega-\omega_0), \quad (1.91)$$
$$\text{or } \int_{-\infty}^{\infty} d\omega e^{i\omega(t-t_0)} = 2\pi\delta(t-t_0). \quad (1.92)$$

This *very important* identity is called an **orthogonality relation**.

C. Inverse Fourier transform

With the help of the orthogonality relation, we can immediately obtain the inverse Fourier transform of $g(\omega)$:

$$g(\omega) = \int_{-\infty}^{\infty} dt f(t)e^{i\omega t}, \quad (1.93)$$
$$\to \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g(\omega)e^{-i\omega t} = \int_{-\infty}^{\infty} dt' f(t')\underbrace{\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{i\omega(t'-t)}}_{=\delta(t-t')}$$
$$= f(t). \quad (1.94)$$

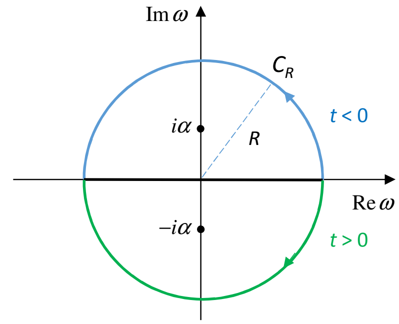

FIG. 7 The integrand in Eq. (1.102) has two poles. One needs to choose a semi-circle C_R appropriately depending on whether $t>0$ or $t<0$.

That is, the Fourier transform and its inverse transform are.

$$g(\omega) = \mathcal{F}f(t) = \int_{-\infty}^{\infty} dt f(t)e^{i\omega t}, \quad (1.95)$$
$$f(t) = \mathcal{F}^{-1}g(\omega) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g(\omega)e^{-i\omega t}. \quad (1.96)$$

You can trace the factor 2π to its origin from the orthogonality relation in Eq. (1.92). It's impossible to remove this factor by rescaling the variables. Some prefer to distribute it equally between two transformations. For example,

$$g(s) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt f(t)e^{ist}, \quad (1.97)$$
$$f(t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} ds g(s)e^{-ist}, \quad (1.98)$$

or

$$g(s) = \int_{-\infty}^{\infty} dt f(t)e^{2\pi ist}, \quad (1.99)$$
$$f(t) = \int_{-\infty}^{\infty} ds g(s)e^{-2\pi ist}. \quad (1.100)$$

We will not adopt these conventions. The 2π factor would always appear in $d\omega/2\pi$.

Ex 4: Given $g(\omega)=\frac{2\alpha}{\omega^2+\alpha^2}$, find out its inverse Fourier transform.

$$f(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{2\alpha}{\omega^2+\alpha^2}e^{-i\omega t} \quad (1.101)$$
$$= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{2\alpha}{(\omega+i\alpha)(\omega-i\alpha)}e^{-i\omega t}. \quad (1.102)$$

This can be evaluated with the help of complex integration. Consider the contour integral,

$$\oint_C = \int_{-\infty}^{\infty} + \int_{C_R}, \quad (1.103)$$

in which C_R a large semi-circle with radius R, as shown in Fig. 7. In order for $\int_{C_R}$ to vanish as $R\to\infty$, if

$t > 0$, then C_R has to go around lower complex plane; if $t < 0$, then it has to go around upper complex plane. In either case, only one pole is within contour C. Using the **residue theorem**, we have

$$f(t) = \begin{cases} e^{-\alpha t} & \text{if } t > 0 \\ 1 & \text{if } t = 0 \\ e^{+\alpha t} & \text{if } t < 0 \end{cases} \quad (1.104)$$

$$= e^{-\alpha|t|}. \quad (1.105)$$

Note that the case with $t = 0$ has been evaluated in Eq. (1.84). This result is consistent with Example 1.

1. Uniqueness of Fourier transform

Lemma 1: If

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g(\omega) e^{i\omega t} = 0, \quad (1.106)$$

then

$$g(\omega) = 0. \quad (1.107)$$

This can be easily proved by performing the inverse transformation to $f(t) = 0$.

Lemma 2: If

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g(\omega) e^{i\omega t} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} h(\omega) e^{i\omega t}, \quad (1.108)$$

then

$$g(\omega) = h(\omega). \quad (1.109)$$

This can be proved by moving the two integrals to the same side, and identify $g - h$ with the g in Lemma 1.

Lemma 2 shows that there cannot be two different functions, $g(\omega), h(\omega)$, that transform to the same function $f(t)$, and vice versa. This is analogous to the expansion of a vector,

$$\mathbf{v} = v_1 \hat{\mathbf{e}}_1 + v_2 \hat{\mathbf{e}}_2 + v_3 \hat{\mathbf{e}}_3. \quad (1.110)$$

If the bases are orthogonal, then the coefficients of expansion are uniquely determined,

$$v_i = \hat{\mathbf{e}}_i \cdot \mathbf{v}. \quad (1.111)$$

Here $\{e^{i\omega t}\}$ plays the role of the orthogonal bases $\{\hat{e}_i\}$, and $g(\omega)$ plays the role of the coefficient of expansion v_i. This is very similar to the discussion in Sec. A3. A major difference is that the dimension of the Hilbert space there is *countably* infinite, whereas it is *uncountably* infinite here.

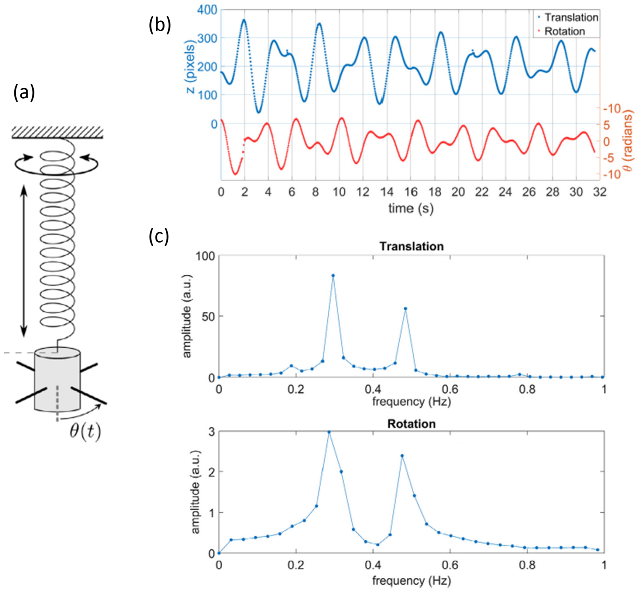

FIG. 8 (a) A Wilberforce pendulum. (b) Vertical displacement and angle of rotation in time. (c) Vertical displacement and angle of rotation in frequency. Figs. from P. Devaux et al, Emergent Scientist **3**, 1 (2019)

D. Spectral analysis

As we have mentioned in Sec. A, if $f(t)$ is a waveform, then its Fourier integral,

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g(\omega) e^{-i\omega t}, \quad (1.112)$$

can be considered as a superposition of numerous harmonic oscillations $\{e^{-i\omega t}\}$. The coefficient $g(\omega)$ is the *weight* of each component. We call it the **frequency distribution**, or the **spectral distribution**, of $f(t)$. Hence Fourier analysis can also be referred to as **spectral analysis**.

The insight we gained from frequency distribution can be very useful. For example, a **Wilberforce pendulum** is a mass suspended by a helical spring (Fig. 8(a)). The displacement $f(t)$ of the pendulum (either vertical or angular) would appear to be irregular (Fig. 8(b)). Its regularity would emerge only if you analyze its frequency distribution $g(\omega)$, which has two peaks from two characteristic frequencies (related to vertical and angular oscillations), see Fig. 8(c).

From Example 2, we learned that

$$f(t) = e^{-\alpha t^2} \;\leftrightarrow\; g(\omega) = \sqrt{\frac{\pi}{\alpha}} e^{-\omega^2/4\alpha}. \quad (1.113)$$

The Fourier transform of a Gaussian peak is also a Gaussian peak. However, if one is broader, then the other is sharper, and vice versa. This is similar to the optical diffraction from a slit. The sharper the slit, the broader

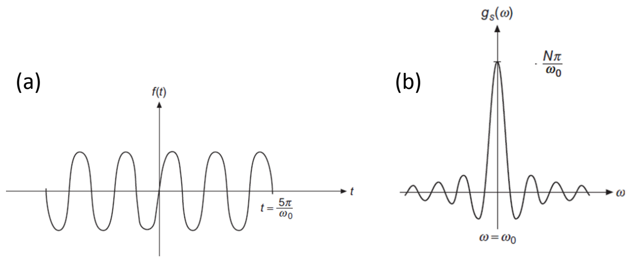

FIG. 9 A finite wave train (a) and its Fourier transform (b).

the diffraction pattern, and vice versa. This is not a coincident, since a diffraction pattern is indeed related to the Fourier transform of its incident wave within the slit (see Zangwill, 2013).

From Example 3, we learned that

$$f(t) = e^{-i\omega_0 t} \;\leftrightarrow\; g(\omega) = 2\pi\delta(\omega - \omega_0). \tag{1.114}$$

This can be considered as an extreme case of the property just mentioned: When a distribution is infinitely sharp, its Fourier transform is flat throughout. Another way to look at this is that, given a simple harmonic oscillation $e^{-i\omega_0 t}$, its spectral distribution contains only *one* single frequency ω_0. Similarly, the spectral distribution of $\sin\omega_0 t = (e^{i\omega_0 t} - e^{-i\omega_0 t})/2i$ would have two delta-peaks at $-\omega_0$ and $+\omega_0$. Note that this is true only for a harmonic oscillation that lasts *forever*. It is *not* so for a *finite* wave train, as explained below.

Ex 5: Given a finite wave train with N oscillations (Fig. 9(a)),

$$f(t) = \begin{cases} \sin\omega_0 t \text{ for } t \in \left[-\frac{NT}{2}.\frac{NT}{2}\right], \; T = \frac{2\pi}{\omega_0}, \\ 0 \quad \text{otherwise.} \end{cases} \tag{1.115}$$

find its spectral distribution $g(\omega)$.

Sol'n:

$$\begin{aligned} g(\omega) &= \int_{-NT/2}^{NT/2} dt \sin\omega_0 t e^{i\omega t} &(1.116)\\ &= \frac{1}{2i}\int_{-NT/2}^{NT/2} dt (e^{i\omega_0 t} - e^{-i\omega_0 t})\, e^{i\omega t} &(1.117)\\ &= i\left[\frac{\sin\frac{NT}{2}(\omega-\omega_0)}{\omega-\omega_0} - \frac{\sin\frac{NT}{2}(\omega+\omega_0)}{\omega+\omega_0}\right]. \end{aligned}$$

This function consists of two peaks, centered at ω_0 and $-\omega_0$. One of the peak centered at ω_0 is shown in Fig. 9(b). The height of the peak $\alpha = NT/2$, and the half-width of the peak $\Delta\omega \simeq 1/\alpha \simeq \omega_0/N$. Thus, if N gets larger, then the peak gets sharper and higher.

Suppose ω_0 is large so that this two peaks are widely separated. Let's focus on one of the peak. It can be shown that the area between the curve $g(\omega)$ and the horizontal axis remains fixed as N changes. First, recall that

$$\int_0^\infty dx\, \frac{\sin x}{x} = \frac{\pi}{2}, \tag{1.118}$$

It follows that, for the peak $g_+(\omega)$ at $+\omega_0$,

$$\begin{aligned} \int_{-\infty}^{\infty} d\omega g_+(\omega) &= i\int_{-\infty}^{\infty} d\omega \frac{\sin\frac{NT}{2}(\omega-\omega_0)}{\omega-\omega_0} &(1.119)\\ &= \pi i. &(1.120) \end{aligned}$$

That is, if we define

$$\delta_\alpha(x) = \frac{1}{\pi}\frac{\sin\alpha x}{x}, \tag{1.121}$$

then

$$\lim_{\alpha\to\infty}\delta_\alpha(x - x_0) = \delta(x - x_0). \tag{1.122}$$

This is the third representation of the delta function being introduced, in addition to the ones in Eqs. (1.86) and (1.87). Finally, when $N \to \infty$,

$$g(\omega) = \pi i\delta(\omega - \omega_0) - \pi i\delta(\omega + \omega_0). \tag{1.123}$$

It can be easily checked that

$$f(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g(\omega)e^{-i\omega t} = \sin\omega_0 t, \tag{1.124}$$

as it should be.

1. Uncertainty relation

Similar to the wave train in Example 5, the function $f(t) = e^{-i\omega_0 t}, t \in [-NT/2, NT/2]$ describes a wave train that lasted $\Delta t = NT$. Its spectral distribution has only one peak at $\omega = \omega_0$ with a width roughly of the order of $\Delta\omega = \omega_0/N$. According to quantum physics, the associated energy uncertainty $\Delta E = \hbar\Delta\omega$. Hence,

$$\Delta E\Delta t \simeq h. \tag{1.125}$$

This is Heisenberg's **uncertainty relation** for energy and time: If a physical events lasts longer, then its energy uncertainty is smaller. On the other hand, if a physics event exists only for a short time, then its energy uncertainty can be large. For example, suppose a laser can emit a beam with a precise period. Nevertheless, if it emits an ultrafast, femto-second pulse, then the energy uncertainty of this pulse can be as large as one electron volt.

Exactly the same analysis applies to the pair of variables (x, k). That is, if $f(x) = e^{ikx}$ describes a wavepacket with an extent $\Delta x = N\lambda$, then its spectral distribution is a peak with a width roughly of the order of $\Delta k = k/N$. The associated momentum uncertainty $\Delta p = \hbar\Delta k$. Hence,

$$\Delta p\Delta x \simeq h. \tag{1.126}$$

This is Heisenberg's uncertainty relation for momentum and position.

2. Fourier transform of multiple variables

Similar to the pair of conjugate variables (t, ω), the Fourier transforms of the conjugate variables (x, k) for position and wavevector are,

$$g(k) = \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \quad (1.127)$$

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} g(k) e^{ikx}. \quad (1.128)$$

Note that we have flipped the signs of the exponents in the kernel by choice, Cf. Eqs. (1.95) and (1.96).

In many cases, the physics described by k is simpler than that described by x. For example, elementary concepts in solid state physics, such as *energy band* and *Fermi surface*, are functions of wavevector, not position.

In general, one can have the following transformations,

$$f(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g(k,\omega) e^{i(kx-\omega t)}, \quad (1.129)$$

$$g(k,\omega) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt f(x,t) e^{-i(kx-\omega t)}. \quad (1.130)$$

That is, a general waveform $f(x,t)$ moving in one dimension can be decomposed as a superposition of $\{e^{i(kx-\omega t)}\}$. The Fourier transforms of $f(t)$ and $f(x)$ can be considered as special cases of $f(x,t)$. This explains why we prefer to choose opposite signs for the exponents in the kernel, $e^{+i\omega t}$ *vs* e^{-ikx}, since we often write a plane wave as $e^{i(kx-\omega t)}$, not as $e^{i(kx+\omega t)}$.

Generalize this to three dimensions, we then have

$$f(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (1.131)$$

$$g(\mathbf{k}) = \int dv f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}, \; dv = d^3r \quad (1.132)$$

in which the integrations are over the whole **k**-space and the whole **r**-space.

In general, for waves travelling in three dimension, we have

$$f(\mathbf{r},t) = \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} g(\mathbf{k},\omega) e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}, \quad (1.133)$$

$$g(\mathbf{k},\omega) = \int dv \int dt f(\mathbf{r},t) e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \quad (1.134)$$

That is, a general waveform $f(\mathbf{r},t)$ moving in three dimension can be decomposed as a superposition of monochromatic plane waves $\{e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\}$.

Ex 6: In 1934, H. Yukawa suggested that the strong nuclear force is mediated by the quantas of nuclear-force field called **mesons**. The nuclear force is short-ranged, with the following form (now called **Yukawa potential**),

$$V(\mathbf{r}) = \frac{e^{-\alpha r}}{r}, \; \alpha > 0. \quad (1.135)$$

Find out its Fourier transform.
Sol'n:

$$V(\mathbf{k}) = \int dv \frac{e^{-\alpha r}}{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (1.136)$$

$$= 2\pi \int_0^{\infty} dr r e^{-\alpha r} \int_0^{\pi} d\cos\theta e^{-ikr\cos\theta} \quad (1.137)$$

$$= \frac{2\pi i}{k} \int_0^{\infty} dr e^{-\alpha r} \left(e^{ikr} - e^{-ikr}\right) \quad (1.138)$$

$$= \frac{4\pi}{k^2 + \alpha^2}. \quad (1.139)$$

If $\alpha \to 0$, then

$$V(\mathbf{k}) = \mathcal{F}\left(\frac{1}{r}\right) = \frac{4\pi}{k^2}. \quad (1.140)$$

This is the Fourier transform of the Coulomb potential in 3D. Note that for the Coulomb potential in 2D, its Fourier transform would be

$$V(\mathbf{k}) = \mathcal{F}\left(\frac{1}{r}\right) = \frac{2\pi}{k}. \quad (1.141)$$

It is left as an exercise to confirm this.

Remarks: The coefficient α is proportional to the mass m of the meson. Therefore, from the range of the nuclear force, which is of the order of fermis, Yukawa estimated the mass of the meson to be around 100 MeVs. Such a particle was first detected in 1947 with a mass of 135 Mev, which is close to the theoretical prediction. Analogously, photons are the quanta of electromagnetic field. If a photon has mass, then the Coulomb potential would also be of the Yukawa form with a tiny non-zero α. Therefore, by detecting any deviation from the inverse square law of the Coulomb force, one can determine whether a photon has a mass or not.

E. Fourier convolution theorem

Consider two functions and their Fourier transforms,

$$f(t) \xrightarrow{\mathcal{F}} \tilde{f}(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{i\omega t}, \quad (1.142)$$

$$g(t) \xrightarrow{\mathcal{F}} \tilde{g}(\omega) = \int_{-\infty}^{\infty} dt g(t) e^{i\omega t}, \quad (1.143)$$

That is,

$$\tilde{f}(\omega) \xrightarrow{\mathcal{F}^{-1}} f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{f}(\omega) e^{-i\omega t}, \quad (1.144)$$

$$\tilde{g}(\omega) \xrightarrow{\mathcal{F}^{-1}} g(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{g}(\omega) e^{-i\omega t}. \quad (1.145)$$

We'd like to find out the inverse transform of their product:

$$\begin{aligned}
&\mathcal{F}^{-1}\left(\tilde{f}(\omega)\tilde{g}(\omega)\right)\\
&= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\tilde{f}(\omega)\tilde{g}(\omega)e^{-i\omega t} \qquad (1.146)\\
&= \int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2 f(t_1)g(t_2)\underbrace{\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{i\omega(t_1+t_2-t)}}_{=\delta(t_1+t_2-t)}\\
&= \int_{-\infty}^{\infty}dt_1 f(t_1)g(t-t_1) \text{ or } \int_{-\infty}^{\infty}dt_2 f(t-t_2)g(t_2)\\
&\equiv (f*g)(t). \qquad (1.147)
\end{aligned}$$

This is called the **convolution integral** of $f(t)$ and $g(t)$. Conversely, we have

$$\mathcal{F}(f*g)(t) = \tilde{f}(\omega)\tilde{g}(\omega). \qquad (1.148)$$

For example, in electromagnetism, the Ohm's law is

$$\mathbf{J}(\omega) = \sigma(\omega)\mathbf{E}(\omega), \qquad (1.149)$$

in which the "$\sim$" has been neglected. Its inverse Fourier transform gives

$$\mathbf{J}(t) = \int_{-\infty}^{\infty}dt'\sigma(t-t')\mathbf{E}(t'). \qquad (1.150)$$

Similarly, in higher dimensions, we have

$$\int\frac{d^3k}{(2\pi)^3}f(\mathbf{k})g(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} = \int dv' f(\mathbf{r}-\mathbf{r}')g(\mathbf{r}'). \qquad (1.151)$$

Conversely, you can check that

$$\int dv f(\mathbf{r})g(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}} = \int\frac{d^3k'}{(2\pi)^3}f(\mathbf{k}-\mathbf{k}')g(\mathbf{k}'). \qquad (1.152)$$

1. Parseval relation

From

$$\begin{aligned}
f(t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\tilde{f}(\omega)e^{-i\omega t}, \qquad (1.153)\\
g(t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\tilde{g}(\omega)e^{-i\omega t}. \qquad (1.154)
\end{aligned}$$

one has

$$\begin{aligned}
&\int_{-\infty}^{\infty}dt f^*(t)g(t)\\
&= \int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega_2}{2\pi}\tilde{f}^*(\omega_1)\tilde{g}(\omega_2)e^{i\omega_1 t-i\omega_2 t}\\
&= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\tilde{f}^*(\omega)\tilde{g}(\omega), \qquad (1.155)
\end{aligned}$$

in which the integral over t gives $2\pi\delta(\omega_1-\omega_2)$. You may consider these integral as an "inner product" between two functions. Then,

$$\langle f(t)|g(t)\rangle = \langle\tilde{f}(\omega)|\tilde{g}(\omega)\rangle. \qquad (1.156)$$

That is, the inner product is invariant under the Fourier transform. Note: For the inner product with frequency integral, we use $\int d\omega/2\pi$, instead of $\int d\omega$.

Ex 7: Suppose there are two charge distributions, $\rho_1(\mathbf{r})$ and $\rho_2(\mathbf{r})$, then the electrostatic potential energy between them is

$$V = \int dv_1\int dv_2\frac{\rho_1(\mathbf{r}_1)\rho_1(\mathbf{r}_2)}{|\mathbf{r}_1-\mathbf{r}_2|}. \qquad (1.157)$$

Write this integral in terms of $\rho_1(\mathbf{k})$ and $\rho_2(\mathbf{k})$, which are Fourier transforms of $\rho_1(\mathbf{r})$ and $\rho_2(\mathbf{r})$.

Sol'n: First, we need

$$\rho(\mathbf{r}) = \int\frac{d^3k}{(2\pi)^3}\rho(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}. \qquad (1.158)$$

Also, from Example 6, we have

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} = \int\frac{d^3k}{(2\pi)^3}\frac{4\pi}{k^2}e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}. \qquad (1.159)$$

It follows that

$$\begin{aligned}
V &= \int dv_1\int dv_2\int\frac{d^3k}{(2\pi)^3}\frac{4\pi}{k^2}\rho_1(\mathbf{r}_1)\rho_2(\mathbf{r}_2)e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\\
&= \int\frac{d^3k}{(2\pi)^3}\frac{4\pi}{k^2}\rho_1(-\mathbf{k})\rho_2(\mathbf{k}) \qquad (1.160)\\
\text{or} &= \int\frac{d^3k}{(2\pi)^3}\frac{4\pi}{k^2}\rho_1^*(\mathbf{k})\rho_2(\mathbf{k}). \qquad (1.161)
\end{aligned}$$

Note that $\rho(-\mathbf{k}) = \rho^*(\mathbf{k})$ if $\rho(\mathbf{r}) \in R$ (see below).

F. Solving differential equations

1. Fourier transform of derivatives

Recall Lemma 2: If

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g(\omega)e^{i\omega t} = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}h(\omega)e^{i\omega t}, \qquad (1.162)$$

then

$$g(\omega) = h(\omega). \qquad (1.163)$$

Now,

$$\begin{aligned}
f(t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g(\omega)e^{-i\omega t}, \qquad (1.164)\\
f^*(t) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}g^*(-\omega)e^{-i\omega t}. \qquad (1.165)
\end{aligned}$$

Therefore, if $f(t)$ is a real-valued function, $f^*(t) = f(t)$, then

$$g^*(\omega) = g(-\omega). \tag{1.166}$$

Similarly,

$$f(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{1.167}$$

$$f^*(\mathbf{r}) = \int \frac{d^3k}{(2\pi)^3} g^*(-\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{1.168}$$

If $f(\mathbf{r})$ is a real-valued function, $f^*(\mathbf{r}) = f(\mathbf{r})$, then

$$g^*(\mathbf{k}) = g(-\mathbf{k}). \tag{1.169}$$

Furthermore, from

$$\frac{df}{dt} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [-i\omega g(\omega)] e^{-i\omega t}, \tag{1.170}$$

we get

$$\mathcal{F}\left(\frac{df}{dt}\right) = -i\omega g(\omega). \tag{1.171}$$

Similarly, from

$$\frac{d^2f}{dt^2} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (-i\omega)^2 g(\omega) e^{-i\omega t}, \tag{1.172}$$

we get

$$\mathcal{F}\left(\frac{d^2f}{dt^2}\right) = (-i\omega)^2 g(\omega). \tag{1.173}$$

Also, from

$$\nabla f = \int \frac{d^3k}{(2\pi)^3} i\mathbf{k} g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{1.174}$$

we get

$$\mathcal{F}(\nabla f) = i\mathbf{k} g(\mathbf{k}). \tag{1.175}$$

Similarly, from

$$\nabla^2 f = \int \frac{d^3k}{(2\pi)^3} i\mathbf{k}\cdot i\mathbf{k} g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{1.176}$$

we get

$$\mathcal{F}\left(\nabla^2 f\right) = -|\mathbf{k}|^2 g(\mathbf{k}). \tag{1.177}$$

From the relations above, we know that under a Fourier transform, a differential operator would become a simple variable. Thus, a linear differential equation for f would become an algebraic equation for g,

$$\mathcal{D}\left(\nabla, \frac{\partial}{\partial t}\right) f(\mathbf{r}, t) = h(\mathbf{r}, t), \tag{1.178}$$

$$\rightarrow D(i\mathbf{k}, -i\omega) g(\mathbf{k}, \omega) = \tilde{h}(\mathbf{k}, \omega), \tag{1.179}$$

in which D is a function with the same form as the differential operator $\mathcal{D}$, and $\tilde{h}$ is the Fourier transform of h.

2. Second-order differential equations

First consider two variables x, y, and write $\psi_{xx} = \partial^2\psi/\partial x^2, \psi_{xy} = \partial^2\psi/\partial x\partial y$ ... etc, then a second-order linear differential equation has the general form,

$$a\psi_{xx} + b\psi_{xy} + c\psi_{yy} + d\psi_x + e\psi_y + f\psi = 0, \tag{1.180}$$

in which the coefficients $a, b, \cdots$ are constants for now. Define $\alpha = b^2 - 4ac$, then depending on the sign of α, a differential equation can be one of three types:

1. $\alpha > 0$: Hyperbolic type, such as the wave equation ($y \rightarrow t$),

$$\frac{\partial^2\psi}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} = 0, \tag{1.181}$$

2. $\alpha = 0$: Parabolic type, such as the diffusion equation ($y \rightarrow t$),

$$D\frac{\partial^2\psi}{\partial x^2} - \frac{\partial\psi}{\partial t} = 0, \tag{1.182}$$

3. $\alpha < 0$: Elliptic type, such as the Laplace equation.

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = 0, \tag{1.183}$$

They are named in such a way because, after Fourier transform, the differential equation becomes,

$$\left(ak_x^2 + bk_xk_y + ck_y^2 + \cdots\right)\tilde{\psi} = 0. \tag{1.184}$$

The quadratic form inside the parenthesis describes a parabola, a hyperbola, or an ellipse on the $k_x - k_y$ plane, depending on the sign of $\alpha = b^2 - 4ac$.

If the coefficients a, b, c are functions of x, y, then depending on the location, the same differential equation can vary from one type to the other. Similar classification can be generalized to linear second-order differential equations with more than two variables (see wiki: partial differential equation).

Ex 8: Solve the wave equation in 1D,

$$\frac{\partial^2\psi}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} = 0, \tag{1.185}$$

with the initial condition (IC),

$$\psi(x, 0) = f(x), \ \frac{\partial\psi(x, 0)}{\partial t} = 0. \tag{1.186}$$

Sol'n: Decompose $\psi(x, t)$ as

$$\psi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\tilde{\psi}(k, t) e^{ikx}, \tag{1.187}$$

$$\text{then } \psi(x, 0) = f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\tilde{\psi}(k, 0) e^{ikx}. \tag{1.188}$$

Fourier transform the wave equation with respect to x, one then has

$$\mathcal{F}_x\left(\frac{\partial^2\psi}{\partial x^2}-\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2}\right) = 0, \quad (1.189)$$

$$\to\ k^2\tilde{\psi}(k,t)+\frac{1}{v^2}\frac{\partial^2\tilde{\psi}}{\partial t^2} = 0. \quad (1.190)$$

The solution is

$$\tilde{\psi}(k,t)=\alpha e^{ikvt}+\beta e^{-ikvt}. \quad (1.191)$$

From the IC, one has

$$\alpha=\beta=\frac{1}{2}\tilde{\psi}(k,0), \quad (1.192)$$

where

$$\tilde{\psi}(k,0)=\int_{-\infty}^{\infty}dx f(x)e^{-ikx}. \quad (1.193)$$

Thus,

$$\begin{aligned}\psi(x,t) &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{1}{2}\tilde{\psi}(k,0)\left(e^{ikvt}+e^{-ikvt}\right)e^{ikx}\\ &= \frac{1}{2}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\tilde{\psi}(k,0)\left[e^{ik(x+vt)}+e^{ik(x-vt)}\right]\\ &= \frac{1}{2}f(x+vt)+\frac{1}{2}f(x-vt). \quad (1.194)\end{aligned}$$

It is an *equal* superposition of a right-moving wave and a left-moving wave because initially the wave has no "velocity", $\partial\psi(x,0)/\partial t=0$.

Ex 9: Solve the diffusion equation in 1D,

$$a^2\frac{\partial^2\psi}{\partial x^2}=\frac{\partial\psi}{\partial t}, \quad (1.195)$$

with the IC $\psi(x,0)=f(x)$. There is no need to know $\partial\psi(x,0)/\partial t$ because the diffusion equation is only first order in time derivative.

Sol'n: Decompose $\psi(x,t)$ as

$$\psi(x,t)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\tilde{\psi}(k,t)e^{ikx}. \quad (1.196)$$

Fourier transform the diffusion equation with respect to x, one then has

$$\mathcal{F}_x\left(a^2\frac{\partial^2\psi}{\partial x^2}\right) = \mathcal{F}_x\left(\frac{\partial\psi}{\partial t}\right) \quad (1.197)$$

$$\to -a^2k^2\tilde{\psi}(k,t) = \frac{\partial\tilde{\psi}}{\partial t}. \quad (1.198)$$

The solution is

$$\tilde{\psi}(k,t)=C(k)e^{-a^2k^2t}. \quad (1.199)$$

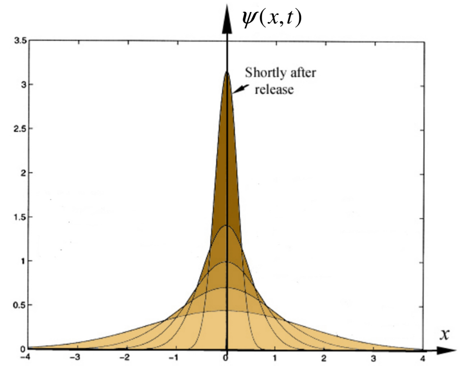

FIG. 10 The profile of diffusion as time evolves.

From the IC, one has

$$\tilde{\psi}(k,0) = \int_{-\infty}^{\infty}dx\psi(x,0)e^{-ikx}, \quad (1.200)$$

$$\text{or } C(k) = \int_{-\infty}^{\infty}dx f(x)e^{-ikx}. \quad (1.201)$$

Finally,

$$\psi(x,t)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}C(k)e^{-a^2k^2t}e^{ikx}. \quad (1.202)$$

This can be calculated if an explicit form of $f(x)$ is given.

For example, suppose

$$\psi(x,0)=f(x)=\delta(x), \quad (1.203)$$

then $C(k)=1$. It follows that

$$\begin{aligned}\psi(x,t) &= \int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{-a^2k^2t}e^{ikx} \quad (1.204)\\ &= \frac{1}{2a\sqrt{2\pi t}}e^{-\frac{x^2}{4a^2t}}=\frac{1}{\sqrt{2\pi}}\frac{1}{\Delta(t)}e^{-\frac{x^2}{\Delta^2(t)}},\end{aligned}$$

where $\Delta(t)\equiv 2a\sqrt{t}$ is the width of the Gaussian distribution. Initially, all particles are located at $x=0$. As time evolves, they diffuse to an extent $\Delta(t)\propto\sqrt{t}$ (Fig. 10). It can be checked that the area below the Gaussian curves (or the total number of particles) remains conserved,

$$\begin{aligned}\int_{-\infty}^{\infty}dx\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\frac{1}{\Delta}\int_{-\infty}^{\infty}e^{-\frac{x^2}{\Delta^2}} \quad (1.205)\\ &= \frac{1}{\sqrt{2\pi}}\frac{1}{\Delta}\sqrt{2\pi}\Delta=1. \quad (1.206)\end{aligned}$$

3. Method of Green function

Consider an inhomogeneous differential equation,

$$\mathcal{D}f(\mathbf{r})=h(\mathbf{r}), \quad (1.207)$$

in which $\mathcal{D}$ is a *linear* differential operator, and $h(\mathbf{r})$ will be referred to as a "source". For example, the Poisson equation in electrostatics is of this form,

$$\nabla^2\phi(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\varepsilon_0}. \tag{1.208}$$

The general source $h(\mathbf{r})$ can be considered as a collection of *point* sources at $\mathbf{r}'$ with weight $h(\mathbf{r}')$,

$$h(\mathbf{r}) = \int dv'\delta(\mathbf{r}-\mathbf{r}')h(\mathbf{r}'). \tag{1.209}$$

Because $\mathcal{D}$ is a *linear operator*, we can first study the effect of one point source,

$$\mathcal{D}G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'), \tag{1.210}$$

then superpose the results from these point sources to obtain $f(\mathbf{r})$,

$$f(\mathbf{r}) = f_0(\mathbf{r}) + \int dv' G(\mathbf{r},\mathbf{r}')h(\mathbf{r}'), \tag{1.211}$$

where f_0 is a solution of the homogeneous equation, $\mathcal{D}f_0 = 0$. It can be checked that

$$\begin{aligned}\mathcal{D}f(\mathbf{r}) &= \mathcal{D}f_0(\mathbf{r}) + \int dv'\mathcal{D}G(\mathbf{r},\mathbf{r}')h(\mathbf{r}') && (1.212)\\ &= \int dv'\delta(\mathbf{r}-\mathbf{r}')h(\mathbf{r}') && (1.213)\\ &= h(\mathbf{r}). && (1.214)\end{aligned}$$

The solution $G(\mathbf{r},\mathbf{r}')$ of a point source is called a **Green function**, and this way of solving a differential equation is called the method of Green function.
Ex 10: Find the Green function of the **Poisson equation** in 3D,

$$\nabla^2 G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{1.215}$$

Sol'n: First, take the Fourier transform of the 3D Poisson equation,

$$\mathcal{F}_{\mathbf{r}}\left[\nabla^2 G(\mathbf{r},\mathbf{r}')\right] = \mathcal{F}_{\mathbf{r}}\left[\delta(\mathbf{r}-\mathbf{r}')\right]. \tag{1.216}$$

Suppose $g(\mathbf{k},\mathbf{r}')$ is the Fourier transform of $G(\mathbf{r},\mathbf{r}')$, then we have

$$\begin{aligned}-k^2 g(\mathbf{k},\mathbf{r}') &= e^{-i\mathbf{k}\cdot\mathbf{r}'}, && (1.217)\\ \to\ g(\mathbf{k},\mathbf{r}') &= -\frac{1}{k^2}e^{-i\mathbf{k}\cdot\mathbf{r}'}. && (1.218)\end{aligned}$$

It follows that

$$\begin{aligned}G(\mathbf{r},\mathbf{r}') &= \int \frac{d^3k}{(2\pi)^3} g(\mathbf{k},\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}} && (1.219)\\ &= -\int \frac{d^3k}{(2\pi)^3}\frac{1}{k^2}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} && (1.220)\\ \cdots &= -\frac{1}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|}. && (1.221)\end{aligned}$$

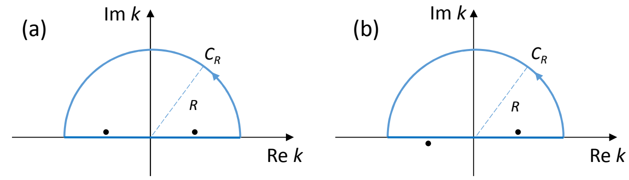

FIG. 11 Two ways to shift the poles off the real axis.

In Eq. (1.208), $h(\mathbf{r})$ can be identified as $-\rho(\mathbf{r})/\varepsilon_0$. Therefore, according to Eq. (1.211), the potential produced by $\rho(\mathbf{r})$ would be

$$\begin{aligned}\phi(\mathbf{r}) &= \int dv'\left(-\frac{1}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right)\left(-\frac{\rho(\mathbf{r}')}{\varepsilon_0}\right) && (1.222)\\ &= \frac{1}{4\pi\varepsilon_0}\int dv'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, && (1.223)\end{aligned}$$

which is a familiar result in electrostatics. There is no need to add an f_0 term since in a space without any charge, $\mathcal{D}f_0 = 0$, the potential would be just a constant.
Ex 11: Find the Green function of the **modified Helmholtz equation** in 3D,

$$(\nabla^2 - k_0^2)G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{1.224}$$

Sol'n: This is similar to the example above. First, take the Fourier transform of both sides, then

$$\begin{aligned}-(k^2+k_0^2)g(\mathbf{k},\mathbf{r}') &= e^{-i\mathbf{k}\cdot\mathbf{r}'}, && (1.225)\\ \to\ g(\mathbf{k},\mathbf{r}') &= -\frac{1}{k^2+k_0^2}e^{-i\mathbf{k}\cdot\mathbf{r}'}. && (1.226)\end{aligned}$$

It follows that

$$\begin{aligned}G(\mathbf{r},\mathbf{r}') &= \int \frac{d^3k}{(2\pi)^3} g(\mathbf{k},\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}} && (1.227)\\ &= -\int \frac{d^3k}{(2\pi)^3}\frac{1}{k^2+k_0^2}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} && (1.228)\end{aligned}$$

It is left as an exercise to calculate this integral and show that

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{e^{-k_0|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}. \tag{1.229}$$

Ex 12: Find the Green function of the **Helmholtz equation** in 3D,

$$(\nabla^2 + k_0^2)G(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'). \tag{1.230}$$

Sol'n: First, take the Fourier transform of both sides, then

$$\begin{aligned}-(k^2-k_0^2)g(\mathbf{k},\mathbf{r}') &= e^{-i\mathbf{k}\cdot\mathbf{r}'}, && (1.231)\\ \to\ g(\mathbf{k},\mathbf{r}') &= -\frac{1}{k^2-k_0^2}e^{-i\mathbf{k}\cdot\mathbf{r}'}. && (1.232)\end{aligned}$$

TABLE I Green functions (see p. 554 in the 5th ed of Mathematical Methods for Physicists, by Arfken and Weber)

	Laplace, ∇^2	Helmholtz, $\nabla^2 + k_0^2$	Modified Helmholtz, $\nabla^2 - k_0^2$
1D	No sol'n	$-\frac{i}{2k}e^{ik\lvert x-x'\rvert}$	$-\frac{1}{2k}e^{-k\lvert x-x'\rvert}$
2D	$\frac{1}{2\pi}\ln\lvert\boldsymbol{\rho}-\boldsymbol{\rho}'\rvert$	$-\frac{i}{4}H_0^{(1)}(k\lvert\boldsymbol{\rho}-\boldsymbol{\rho}'\rvert)$	$-\frac{1}{2\pi}K_0(k\lvert\boldsymbol{\rho}-\boldsymbol{\rho}'\rvert)$
3D	$-\frac{1}{4\pi}\frac{1}{\lvert\mathbf{r}-\mathbf{r}'\rvert}$	$-\frac{1}{4\pi}\frac{e^{ik_0\lvert\mathbf{r}-\mathbf{r}'\rvert}}{\lvert\mathbf{r}-\mathbf{r}'\rvert}$	$-\frac{1}{4\pi}\frac{e^{-k_0\lvert\mathbf{r}-\mathbf{r}'\rvert}}{\lvert\mathbf{r}-\mathbf{r}'\rvert}$

It follows that

$$\begin{aligned} G(\mathbf{r},\mathbf{r}') &= \int \frac{d^3k}{(2\pi)^3} g(\mathbf{k},\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}} && (1.233)\\ &= -\int \frac{d^3k}{(2\pi)^3}\frac{1}{k^2-k_0^2}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')},\ \lvert\mathbf{r}-\mathbf{r}'\rvert \equiv R \\ &= -\frac{1}{(2\pi)^2 iR}\int_0^\infty \frac{kdk}{k^2-k_0^2}\left(e^{ikR}-e^{-ikR}\right) \\ &= -\frac{1}{(2\pi)^2 iR}\int_{-\infty}^\infty \frac{kdk}{k^2-k_0^2}e^{ikR}. && (1.234)\end{aligned}$$

There are two poles along the real axis, and there are several ways to avoid them, which would give different results. Some physics judgement is required to pick up a valid answer.

For example, in Fig. 11(a), both poles are shifted *upward* to $\pm k_0 + i\varepsilon$. To evaluate the integral in Eq. (1.234), consider an integral around a closed contour C,

$$\underbrace{\int_{-\infty}^{\infty}}_{\equiv I} + \int_{C_R} = \oint_C = 2\pi i \sum \text{Res}. \tag{1.235}$$

The integral over C_R is zero as $R \to \infty$. Thus,

$$\begin{aligned} I &= \oint_C \frac{kdk}{(k+k_0)(k-k_0)}e^{ikR} && (1.236)\\ &= 2\pi i\left(\frac{-k_0}{-2k_0}e^{-ik_0R} + \frac{k_0}{2k_0}e^{+ik_0R}\right) && (1.237)\\ &= 2\pi i \cos k_0 R. && (1.238)\end{aligned}$$

Hence,

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{2\pi R}\cos k_0 R. \tag{1.239}$$

On the other hand, if both poles are shifted *downward* to $\pm k_0 - i\varepsilon$, then there is no pole inside C and the integral is zero. Hence $G(\mathbf{r},\mathbf{r}') = 0$, which is clearly not a good answer.

It is also possible to move the pole at $-k_0$ downward and the one at $+k_0$ upward, $k_0^2 \to k_0^2 + i\varepsilon$, as shown in Fig. 11(b). It follows that

$$\begin{aligned} I &= 2\pi i\left(0 + \frac{k_0}{2k_0}e^{+ik_0R}\right) && (1.240)\\ &= \pi i e^{+ik_0R}. && (1.241)\end{aligned}$$

This leads to

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi R}e^{+ik_0R}. \tag{1.242}$$

On the other hand, if we move the pole at $-k_0$ upward and the one at $+k_0$ downward, $k_0^2 \to k_0^2 - i\varepsilon$, then

$$\begin{aligned} I &= 2\pi i\left(\frac{-k_0}{-2k_0}e^{-ik_0R} + 0\right) && (1.243)\\ &= \pi i e^{-ik_0R}. && (1.244)\end{aligned}$$

This leads to

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi R}e^{-ik_0R}. \tag{1.245}$$

We now have three results from Eqs. (1.239), (1.242), and (1.245). If you combine it with $e^{-i\omega t}$, then $e^{\pm ik_0R}e^{-i\omega t}/R = e^{\pm i(k_0R\mp\omega t)}/R$ represent outgoing and incoming spherical waves, while the first solution in Eq. (1.239) has both. The boundary condition of the physics problem would tell you which one to keep. In most cases, the spherical wave is propagating outward, so we should pick the one in Eq. (1.242).

Note: If you do not move the poles away from the real axis, but choose a contour C that walks around the poles with a tiny semi-circle (again there are 4 ways to do that), then you'll get a result different from the ones above. This is not a valid approach.

Finally, some more Green functions in lower dimensions can be found in Table I.

G. Connection between Fourier series and Fourier integral

Finally, we comment on the connection between Fourier series and Fourier integral. The former deals with periodic functions, whereas the latter does not have such a restriction. In physics, to avoid the divergence of field-related quantities due to an infinite space, we would sometimes contain a system in a box. The space is expanded to be infinite only at the end of a calculation. This is called **box normalization**. If the **periodic boundary condition** (PBC) is imposed, then any physical quantity that is originally non-periodic in space would become periodic. Thus, Fourier series and Fourier

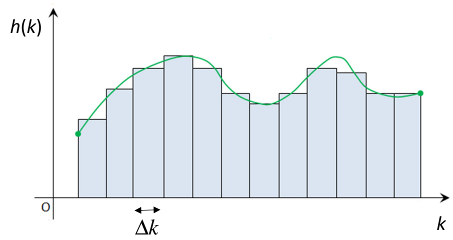

FIG. 12 A function $h(k)$ with discrete variables k_n.

integral should be closely related when $L \to \infty$, as we'll show.

Let's consider a 1D box with PBC. A wave e^{ikx} inside has to satisfy the PBC,

$$e^{ik(x+L)} = e^{ikx}. \tag{1.246}$$

As a result, the wave vectors are discrete,

$$e^{ikL} = 1, \text{ or } k_n = \frac{2\pi}{L} n, n \in Z. \tag{1.247}$$

This wave can be, e.g., an EM wave (in the study of blackbody radiation), or an electron wave (in the study of electron gas) etc. We can superpose these waves with different k_n's to build a general waveform,

$$f(x) = \frac{1}{L} \sum_{k_n} g(k_n) e^{ik_n x}. \tag{1.248}$$

Obviously this satisfies $f(x+L) = f(x)$. With the orthogonality relation,

$$\int_{-L/2}^{L/2} dx e^{-ik_n x} e^{ik_m x} = L\delta_{nm}, \tag{1.249}$$

we can get the coefficients of expansion,

$$g(k_n) = \int_{-L/2}^{L/2} dx f(x) e^{-ik_n x}. \tag{1.250}$$

Now, to discuss a wave in an infinite space, we need to let $L \to \infty$. It follows that $\Delta k_n = 2\pi/L \to 0$. That is k_n approaches a continuous variable k, and $g(k_n)$ approaches a continuous function $g(k)$. In a graph (see Fig. 12), the summation

$$A = \sum_{k_n} \Delta k \; h(k_n), \;\; \Delta k_n = \frac{L}{2\pi}. \tag{1.251}$$

represents the sum of the areas of rectangles with width Δk and height $h(k_n)$. When Δk is very small, this area approaches the area below the curve $h(k)$,

$$\sum_{k_n} \Delta k \; h(k_n) \xrightarrow{L \gg 1} \int dk h(k). \tag{1.252}$$

Alternatively, one can write

$$\sum_{k_n} h(k_n) = \frac{1}{\Delta k} \sum_{k_n} \Delta k h(k_n) \tag{1.253}$$

$$\xrightarrow{L \gg 1} \frac{L}{2\pi} \int dk h(k). \tag{1.254}$$

Thus,

$$f(x) = \frac{1}{L} \sum_{k_n} g(k_n) e^{ik_n x}, \tag{1.255}$$

$$\xrightarrow{L \gg 1} f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} g(k) e^{ikx}. \tag{1.256}$$

Also,

$$g(k_n) = \int_{-L/2}^{L/2} dx f(x) e^{-ik_n x}, \tag{1.257}$$

$$\xrightarrow{L \gg 1} g(k) = \int_{-\infty}^{\infty} dx f(x) e^{-ikx} \tag{1.258}$$

Furthermore, there are two versions of the orthogonality relation: one discrete, the other continuous. To connect these two, we need to connect in some way Kronecker delta function with Dirac delta function. This can be done as follows: To discretize a continuous variable k, we can chop it to pieces, each with size Δk, so that

$$\delta_{nm} \simeq \delta\left(\frac{k}{\Delta k} - \frac{k'}{\Delta k}\right) \tag{1.259}$$

$$= \Delta k \delta(k - k') \tag{1.260}$$

$$= \frac{2\pi}{L} \delta(k - k'). \tag{1.261}$$

As a result, the discrete version in Eq. (1.249),

$$\int_{-\infty}^{\infty} dx e^{i(k-k')x} = 2\pi\delta(k - k'), \tag{1.262}$$

$$\xrightarrow{L \gg 1} \int_{-L/2}^{L/2} dx e^{-ik_n x} e^{ik_m x} = L\delta_{nm}. \tag{1.263}$$

1. Higher dimensions

The correspondence above can be generalized to (two or) three dimensions. The space is a cubic box with length L. Because of the PBC, the wave vectors are discrete,

$$\mathbf{k} = \frac{2\pi}{L} n\hat{\mathbf{x}} + \frac{2\pi}{L} l\hat{\mathbf{y}} + \frac{2\pi}{L} l\hat{\mathbf{z}}, \;\; n, m, l \in Z$$

$$\text{and } \Delta^3 k = \left(\frac{2\pi}{L}\right)^3 = \frac{(2\pi)^3}{V}. \tag{1.264}$$

In the discrete version,

$$f(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{1.265}$$

With the correspondence,

$$\sum_{\mathbf{k}} h(\mathbf{k}) \longleftrightarrow \int \frac{d^3\mathbf{k}}{\Delta^3 k} h(\mathbf{k}) = V \int \frac{d^3 k}{(2\pi)^3} h(\mathbf{k}), \quad (1.266)$$

one has

$$f(\mathbf{r}) = \int \frac{d^3 k}{(2\pi)^3} g(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (1.267)$$

To convert between two orthogonality relations, one can use,

$$\begin{aligned} \delta_{\mathbf{k},\mathbf{k}'} \longleftrightarrow \quad & \delta^3\left(\frac{\mathbf{k}}{\Delta k} - \frac{\mathbf{k}'}{\Delta k}\right) & (1.268) \\ = \; & \Delta^3 k \; \delta^3(\mathbf{k} - \mathbf{k}'). & (1.269) \end{aligned}$$

Note that the $\mathbf{k}$'s on the LHS (RHS) of the equation are discrete (continuous). The orthogonality relation for discrete variables is

$$\int_{\text{box}} dv e^{-i\mathbf{k}'\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} = V \delta_{\mathbf{k},\mathbf{k}'}. \quad (1.270)$$

When $L \to \infty$, it becomes

$$\int_{\text{whole}} dv e^{-i\mathbf{k}'\cdot\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} = (2\pi)^3 \delta(\mathbf{k} - \mathbf{k}'). \quad (1.271)$$

Finally, the inverse transforms for discrete $\mathbf{k}$ and continuous $\mathbf{k}$ have the same form,

$$\begin{aligned} g(\mathbf{k}) \; &= \; \int_{\text{box}} dv f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}, & (1.272) \\ \text{and } g(\mathbf{k}) \; &= \; \int_{\text{whole}} dv f(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}. & (1.273) \end{aligned}$$

H. Poisson summation formula

Suppose $f(x)$ is a *localized* function. That is, it decays exponentially when $|x| \gg 1$. Its Fourier transform and inverse Fourier transform are

$$\begin{aligned} f(x) \; &= \; \int_{-\infty}^{\infty} \frac{dk}{2\pi} \tilde{f}(k) e^{ikx}, & (1.274) \\ \tilde{f}(k) \; &= \; \int_{-\infty}^{\infty} dx f(x) e^{-ikx}. & (1.275) \end{aligned}$$

Consider the following **lattice sum** of $f(x)$,

$$F(x) = \sum_{n=-\infty}^{\infty} f(x + na). \quad (1.276)$$

Since $F(x)$ is a periodic function, $F(x + a) = F(x)$, it can be expanded as a Fourier series,

$$F(x) = \sum_{n=-\infty}^{\infty} F_n e^{2\pi i n/a x}. \quad (1.277)$$

The coefficients of expansion,

$$\begin{aligned} F_n \; &= \; \frac{1}{a} \int_0^a dx F(x) e^{-2\pi i n/a x} & (1.278) \\ &= \; \frac{1}{a} \sum_{m=-\infty}^{\infty} \int_0^a dx f(x + ma) e^{-2\pi i n/a x} & (1.279) \\ &= \; \frac{1}{a} \sum_{m=-\infty}^{\infty} \int_{ma}^{(m+1)a} dx f(x) e^{-2\pi i n/a x} \underbrace{e^{2\pi i n m}}_{=1} & \\ &= \; \frac{1}{a} \int_{-\infty}^{\infty} dx f(x) e^{-2\pi i n/a x} & (1.280) \\ &= \; \frac{1}{a} \tilde{f}(k_n), \;\; k_n \equiv \frac{2\pi}{a} n & (1.281) \end{aligned}$$

where $\tilde{f}$ is given in Eq. (1.275). Substitute this result to the F_n in Eq. (1.277), then the lattice sum

$$\sum_{n=-\infty}^{\infty} f(x + na) = \frac{1}{a} \sum_{n=-\infty}^{\infty} \tilde{f}(k_n) e^{2\pi i n/a x}. \quad (1.282)$$

This is the **Poisson summation formula**, which relates the lattice sum of $f(x)$ to the lattice sum of $\tilde{f}(k_n)$.

Recall that if $f(x)$ is a broad distribution, then $\tilde{f}(k)$ is sharp, and vice versa. So if $f(x)$ is broad, then the lattice sum of $\tilde{f}(k_n)$ would converge quickly, or the other way around. As an extreme case, take $f(x) = \delta(x)$, then $\tilde{f}(k) = 1$, and

$$\sum_{n=-\infty}^{\infty} \delta(x + na) = \frac{1}{a} \sum_{n=-\infty}^{\infty} e^{2\pi i n/a x}. \quad (1.283)$$

Such a summation appears in the theory of crystal diffraction (see Chap 2 of Kittel): The coherent superposition of diffracted waves on the RHS gives rise to the diffraction peaks on the LHS.

Let's consider two special cases:

1) Take $x = 0$, then one has

$$\sum_{n=-\infty}^{\infty} f(na) = \frac{1}{a} \sum_{m=-\infty}^{\infty} \tilde{f}(k_n). \quad (1.284)$$

Suppose $f(x) \in R$, then $f(-k) = f^*(k)$. Decompose the summation on the RHS, such that

$$\begin{aligned} \sum_{n=-\infty}^{\infty} \tilde{f}(k_n) \; &= \; \tilde{f}(0) + \sum_{n=1}^{\infty} \tilde{f}(k_n) + \sum_{n=1}^{\infty} \tilde{f}(-k_n) & \\ &= \; \tilde{f}(0) + 2\text{Re} \sum_{n=1}^{\infty} \tilde{f}(k_n) & (1.285) \end{aligned}$$

It follows that

$$a \sum_{n=-\infty}^{\infty} f(na) = \underbrace{\int_{-\infty}^{\infty} dx f(x)}_{=\tilde{f}(0)} + 2\text{Re} \sum_{n=1}^{\infty} \tilde{f}(k_n). \quad (1.286)$$

When $a \to 0$, the LHS should approach the integral on the RHS, since both are the area bounded between the curve $f(x)$ and the x-axis (see Fig. 12). That is, the summation over $\tilde{f}(k_n)$ ($\to 0$ since $k_n = 2\pi n/a \gg 1$) on the RHS should approach zero (see Modern Condensed Matter Physics, by Girvin and Yang). For a finite a, one can use this formula to evaluate a summation with an integral, plus a controllable correction.

2) Take $x = a/2$, then one has

$$\sum_{n=-\infty}^{\infty} f\left(na + \frac{a}{2}\right) = \frac{1}{a} \sum_{m=-\infty}^{\infty} \tilde{f}(k_n) e^{\pi i n}. \qquad (1.287)$$

Suppose $f(-x) = f(x)$, then the LHS

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} f\left(na + \frac{a}{2}\right) && (1.288)\\ =\ & f\left(\frac{a}{2}\right) + \sum_{n=1}^{\infty} f\left(na + \frac{a}{2}\right) + \sum_{n=1}^{\infty} f\left(-na + \frac{a}{2}\right) \\ =\ & 2\sum_{n=0}^{\infty} f\left(na + \frac{a}{2}\right). && (1.289)\end{aligned}$$

On the RHS, one has

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} \tilde{f}(k_n) e^{\pi i n} && (1.290)\\ =\ & \tilde{f}(0) + \sum_{n=1}^{\infty} (-1)^n \tilde{f}(k_n) + \sum_{n=1}^{\infty} (-1)^n \tilde{f}(-k_n) \\ =\ & \tilde{f}(0) + 2\mathrm{Re} \sum_{n=1}^{\infty} (-1)^n \tilde{f}(k_n). && (1.291)\end{aligned}$$

Combining these two equations, one then has

$$\begin{aligned} & a\sum_{n=0}^{\infty} f\left(na + \frac{a}{2}\right) && (1.292)\\ =\ & \frac{\tilde{f}(0)}{2} + \mathrm{Re} \sum_{n=1}^{\infty} (-1)^n \tilde{f}(k_n) \qquad \text{Cf. } Eq.\ 1.286 \\ =\ & \int_0^{\infty} dx f(x) + 2\sum_{n=1}^{\infty} (-1)^n \int_0^{\infty} dx f(x) \cos\frac{2\pi n}{a} x. \end{aligned}$$

This has been used in the theory of de Haas-van Alphen effect, in which one has to sum over Landau-level energies (see Principles of the Theory of Solids, by Ziman).

1. Casimir effect

The ground state energy of a simple harmonic oscillator is $\hbar\omega/2$, which is the **zero-point energy**. The oscillating mass cannot have both $x = 0$ and $p = 0$ since this would violate the uncertainty principle. Similar zero-point energies exist in the oscillation of electromagnetic field. An EM wave has the energy dispersion $\omega_k = ck$, and the zero-point energy for **k**-mode is $\hbar\omega_k/2$. Since the number of oscillation modes is infinite, total zero-point energy diverges,

$$E_0 = 2\sum_{\mathbf{k}} \frac{1}{2}\hbar\omega_k \to \infty. \qquad (1.293)$$

The factor 2 comes from *two* polarizations for each **k**-mode.

In the presence of two parallel, infinite metal plates, the modes of oscillations would be altered. As a result, the zero-point energy between the plates would be slightly different. This results in an interaction between two metal plates (the **Casimir effect**). We now calculate this Casimir force with the help of the Poisson summation formula (Lin, College Physics, **27**, 9 (2008)).

Suppose the two plates are separated with a distance a. The modes within the plates have the wavevectors

$$\mathbf{k} = \left(k_x, k_y, \frac{n\pi}{a}\right),\ k_x, k_y \in R,\ n = 0, 1, 2\cdots. \qquad (1.294)$$

Without the plates, k_z would be continuous. This is the source of the energy difference between these two setups.

First, without the plates, total zero-point energy

$$\begin{aligned} E_0 &= \sum_{\mathbf{k}} \hbar\omega_k,\ \omega_k = ck && (1.295)\\ &= \hbar c V \int \frac{d^3k}{(2\pi)^3} k && (1.296)\\ &= \frac{\hbar c V}{(2\pi)^3} \int d^2k_\parallel dk_z \sqrt{k_\parallel^2 + k_z^2},\ k_z \to \frac{\pi}{a} x && (1.297)\\ &= \frac{\hbar c V}{(2\pi)^2} \int_0^{\infty} k_\parallel dk_\parallel \int_{-\infty}^{\infty} \frac{\pi}{a} dx \sqrt{k_\parallel^2 + \left(\frac{\pi}{a}x\right)^2}. && (1.298)\end{aligned}$$

On the other hand, with the plates,

$$\begin{aligned} E_0' &= \sum_{\mathbf{k}_\parallel} \sum_{k_z} \hbar\omega_k,\ k_z = \frac{\pi}{a} n && (1.299)\\ &= \hbar c S \int \frac{d^2k_\parallel}{(2\pi)^2} \sum_{k_z} \sqrt{k_\parallel^2 + k_z^2},\ V = Sa && (1.300)\\ &= \frac{\hbar c S}{2\pi} \int_0^{\infty} k_\parallel dk_\parallel \left[\frac{1}{2}k_\parallel + \sum_{n=1}^{\infty} \sqrt{k_\parallel^2 + \left(\frac{\pi}{a} n\right)^2}\right]. && (1.301)\end{aligned}$$

The $n = 0$ mode is taken out of the summation and is divided by 2 because this mode has only *one* polarization (parallel to the plate).

Both Eqs. (1.298) and (1.301) have similar integrands. Define

$$f(x) = \int_0^{\infty} kdk \sqrt{k^2 + \left(\frac{\pi}{a}x\right)^2}, \qquad (1.302)$$

where $k_\parallel$ is simply written as k. then

$$E_0 = \frac{\hbar c S}{4\pi}\int_{-\infty}^{\infty} dx f(x), \quad (1.303)$$

$$E_0' = \frac{\hbar c S}{2\pi}\left[\frac{f(0)}{2} + \sum_{n=1}^{\infty} f(n)\right]. \quad (1.304)$$

From Eq. (1.286), one has

$$f(0) + 2\sum_{n=1}^{\infty} f(n) = 2\int_0^{\infty} dx f(x) + 2\mathrm{Re}\sum_{n=1}^{\infty}\tilde{f}(k_n). \quad (1.305)$$

It follows that ($\Delta E \equiv E_0' - E_0$)

$$\frac{\Delta E}{S} = \frac{\hbar c}{2\pi}\left[\frac{f(0)}{2} + \sum_{n=1}^{\infty} f(n) - \int_0^{\infty} dx f(x)\right] \quad (1.306)$$

$$= \frac{\hbar c}{2\pi}\mathrm{Re}\sum_{n=1}^{\infty}\tilde{f}(k_n) \quad (1.307)$$

$$= \frac{\hbar c}{2\pi}\sum_{n=1}^{\infty}\int_0^{\infty} kdk\int_{-\infty}^{\infty} dx\sqrt{k^2 + \left(\frac{\pi}{a}x\right)^2}\cos(2\pi n x).$$

The force per unit area between plates is given by the gradient of energy, $F = \frac{d\Delta E/S}{da}$, hence

$$F = \frac{\hbar c}{2\pi}\sum_{n=1}^{\infty}\int_0^{\infty} kdk\int_{-\infty}^{\infty} dx\frac{-\frac{\pi^2}{a^3}x^2}{\sqrt{k^2 + \left(\frac{\pi}{a}x\right)^2}}\cos(2\pi n x)$$

$$= -\frac{\hbar c}{\pi^2}\sum_{n=1}^{\infty}\int_0^{\infty} kdk\underbrace{\int_0^{\infty} du\frac{u^2}{\sqrt{k^2+u^2}}\cos(2nau)}_{\equiv I},$$

in which $u \equiv \frac{\pi}{a}x$. We can write

$$\cos(2nau) = -\frac{1}{(2nu)^2}\frac{d^2}{da^2}\cos(2nau), \quad (1.308)$$

then the integral

$$I = -\frac{1}{(2n)^2}\frac{d^2}{da^2}\underbrace{\int_0^{\infty} du\frac{\cos(2nau)}{\sqrt{k^2+u^2}}}_{=K_0(2nak)}, \quad (1.309)$$

The following identify has been used to get the Hankel function (see e.g., the 5th ed. of Mathematical Methods for Physicists, by Arfken and Weber),

$$K_0(x) = \int_0^{\infty} dv\frac{\cos xv}{\sqrt{1+v^2}}. \quad (1.310)$$

It follows that

$$F = \frac{\hbar c}{4\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\int_0^{\infty} kdk\frac{d^2}{da^2}K_0(2nak). \quad (1.311)$$

From the identity

$$\int_0^{\infty} dx x K_0(\alpha x) = \frac{1}{\alpha^2}, \quad (1.312)$$

we finally have

$$F(a) = \frac{\hbar c}{4\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\frac{d^2}{da^2}\frac{1}{4n^2a^2} \quad (1.313)$$

$$= \frac{6\hbar c}{16\pi^2}\frac{1}{a^4}\underbrace{\sum_{n=1}^{\infty}\frac{1}{n^4}}_{=\pi^4/90} \quad (1.314)$$

$$= \frac{\pi^2}{240}\frac{\hbar c}{a^4} \simeq \frac{0.01}{(\frac{a}{\mu\mathrm{m}})^4}\frac{\mathrm{dyn}}{\mathrm{cm}^2}. \quad (1.315)$$

This is an attractive force. For a experimental demonstration, see Lamoreaux, Phys. Rev. Lett. **78**, 5 (1997). The Casimir force is not necessarily attractive, however. It can be repulsive, for example, if one of the plate is replaced by a dielectric.