From Fourier Series to Fourier Integral

Fourier series for periodic functions

Consider the space of doubly differentiable functions of one variable x defined within the interval $x \in [-L/2, L/2]$. In this space, Laplace operator is Hermitian and its eigenfunctions $\{e_n(x)\}$, defined as

$$\frac{\partial^2 e_n}{\partial x^2} = \lambda_n\, e_n \; , \tag{1}$$

$$e_n(L/2) = e_n(-L/2) \; , \qquad e_n'(L/2) = e_n'(-L/2) \tag{2}$$

form an ONB. With an exception for $\lambda = 0$, each eigenvalue λ turns out to be doubly degenerate, so that there are many ways of choosing the ONB. Let us consider

$$e_n(x) = e^{ik_n x}/\sqrt{L} \; , \tag{3}$$

$$\lambda_n = -k_n^2, \qquad k_n = \frac{2\pi n}{L} \; , \qquad n = 0, \pm 1, \pm 2, \dots \; . \tag{4}$$

For any function $f(x) \in \mathcal{L}_2[-L/2, L/2]$, the Fourier series with respect to the ONB $\{e_n(x)\}$ is

$$f(x) = \sum_{n=-\infty}^{\infty} \langle e_n | f \rangle | e_n \rangle = L^{-1/2} \sum_{n=-\infty}^{\infty} f_n\, e^{ik_n x} \; , \tag{5}$$

where

$$f_n = \langle e_n | f \rangle = L^{-1/2} \int_{-L/2}^{L/2} f(x) e^{-ik_n x} dx \; . \tag{6}$$

In practice, it is not convenient to keep the factor $L^{-1/2}$ in both relations. We thus redefine f_n as $f_n \to L^{-1/2} f_n$ to get

$$f(x) = L^{-1} \sum_{n=-\infty}^{\infty} f_n\, e^{ik_n x} \; , \tag{7}$$

$$f_n = \int_{-L/2}^{L/2} f(x) e^{-ik_n x} dx \; . \tag{8}$$

If $f(x)$ is real, the series can be actually rewritten in terms of sines and cosines. To this end we note that from (8) it follows that

$$f_{-n} = f_n^* \; , \qquad \text{if} \quad \operatorname{Im} f(x) \equiv 0 \; , \tag{9}$$

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and we thus have

$$f(x) = \frac{f_0}{L} + L^{-1} \sum_{n=1}^{\infty} [f_n\, e^{ik_n x} + f_n^*\, e^{-ik_n x}] = \frac{f_0}{L} + \frac{2}{L} \sum_{n=1}^{\infty} \mathrm{Re}\, f_n\, e^{ik_n x} \ . \quad (10)$$

Now if we parameterize

$$f_n = A_n - iB_n \ , \quad (11)$$

where A_n and B_n are real and plug this parametrization in (8) and (10), we get

$$f(x) = \frac{f_0}{L} + \frac{2}{L} \sum_{n=1}^{\infty} [\, A_n \cos k_n x \, + \, B_n \sin k_n x\,] \ , \quad (12)$$

where

$$A_n = \int_{-L/2}^{L/2} f(x)\cos k_n x\, dx \ , \qquad B_n = \int_{-L/2}^{L/2} f(x)\sin k_n x\, dx \ . \quad (13)$$

Eqs. (12)-(13)—and also Eq. (11)—hold true even in the case of complex $f(x)$, with the reservation that now A_n and B_n are complex.

Actually, the function $f(x)$ should not necessarily be L-periodic. For non-periodic functions, however, the convergence will be only in the sense of the inner-product norm. For non-periodic functions the points $x = \pm L/2$ can be considered as the points of discontinuity, in the vicinity of which the Fourier series will demonstrate the Gibbs phenomenon.

Fourier integral

If $f(x)$ is defined for any $x \in (-\infty, \infty)$ and is well behaved at $|x| \to \infty$, we may take the limit of $L \to \infty$. The result will be the *Fourier integral*:

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, f_k\, e^{ikx} \ , \quad (14)$$

$$f_k = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \ . \quad (15)$$

Indeed, at very large L we can take the limit $L \to \infty$ in (8):

$$f_n = \int_{-L/2}^{L/2} f(x) e^{-ik_n x} dx \ \rightarrow \ \int_{-\infty}^{\infty} f(x) e^{-ik_n x} dx \ . \quad (16)$$

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Then, we consider (7) as an integral sum corresponding to a continuous variable k, so that k_n are just the discrete points where the function is calculated:

$$f(x) = L^{-1} \sum_{n=-\infty}^{\infty} f_n\, e^{ik_n x} = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} f_{k_n}\, e^{ik_n x}\, \Delta k \,, \qquad (17)$$

where $\Delta k = k_{n+1} - k_n = 2\pi/L$, and f_k is given by (16) In the limit of $L \to \infty$, we have $\Delta k \to 0$, and the integral sum approaches the integral:

$$\sum_{n=-\infty}^{\infty} f_{k_n}\, e^{ik_n x}\, \Delta k \;\to\; \int_{-\infty}^{\infty} f_k\, e^{ikx}\, dk \,. \qquad (18)$$

The function $g(k) \equiv f_k$ is called *Fourier transform* of the function f. Apart from the factor $1/2\pi$ and the opposite sign of the exponent—both being matters of definition—the functions f and g enter the relations (14)-(15) symmetrically. This means that if g is the Fourier transform of f, then f is the Fourier transform of g, up to a numeric factor and different sign of the argument. By this symmetry it is seen that the representation of any function f in the form of the Fourier integral (14) is *unique*. Indeed, given Eq. (14) with *some f_k*, we can treat f as a Fourier transform of $g(k) \equiv f_k$, which immediately implies that f_k should obey (15) and thus be unique for the given f. For a real function f the uniqueness of the Fourier transform immediately implies

$$f_{-k} = f_k^* \,, \qquad (19)$$

by complex-conjugating Eq. (14).

Application to Linear PDE

The application of the Fourier integral to linear PDE's is based on the fact that Fourier transform turn differentiation into simple algebraic operations. Indeed, if

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, f_k\, e^{ikx} \,, \qquad (20)$$

then, differentiating under the sign of the integral, we get

$$f'(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, ik\, f_k\, e^{ikx} \,, \qquad (21)$$

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$$f''(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \, (-k^2) \, f_k \, e^{ikx} \;, \tag{22}$$

and so forth. As a characteristic example, consider the heat equation on the infinite x-axis

$$u_t = u_{xx} \;, \qquad\qquad x \in (-\infty, \, \infty) \;, \tag{23}$$

with some given initial condition $u(x, 0)$. Let us look for the solution in the form of the Fourier integral

$$u(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \, g(k, t) \, e^{ikx} \;. \tag{24}$$

[Note the analogy with looking for the solution in the form of the Fourier series when solving boundary value problems.] Plugging this into Eq. (23) we get

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \, [\dot{g} + k^2 g] \, e^{ikx} \; = \; 0 \;, \tag{25}$$

and by uniqueness of the Fourier integral immediately conclude that

$$\dot{g} + k^2 g \; = \; 0 \;. \tag{26}$$

That is we replaced PDE with an ordinary differential equation for the Fourier transform. This equation is readily solved:

$$g(k, t) \; = \; g(k, 0) \, e^{-k^2 t} \;, \tag{27}$$

where the initial condition $g(k, 0)$ is found by Fourier transforming the function $u(x, 0)$:

$$g(k, 0) = \int_{-\infty}^{\infty} dx \, u(x, 0) \, e^{-ikx} \;. \tag{28}$$

The final answer comes in the form of the integral

$$u(x, t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \, g(k, 0) \, e^{-k^2 t + ikx} \;. \tag{29}$$

As an important example, let us find the simplest non-trivial (that is not identically constant in the real space) solution. To this end we set $g(k, 0) = c$, where c is just a constant, and get

$$u(x, t) = c \int_{-\infty}^{\infty} \frac{dk}{2\pi} \, e^{-k^2 t + ikx} \;. \tag{30}$$

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The integral we are dealing with is the famous Gaussian integral

$$\int_{-\infty}^{\infty} e^{-ay^2+by}\, dy \;=\; \sqrt{\frac{\pi}{a}}\; e^{b^2/4a} \;. \tag{31}$$

The above expression is valid for any complex number b and for all complex a's for which $\operatorname{Re} a > 0$. Moreover, this formula remains valid if $\operatorname{Re} a = 0$, provided $\operatorname{Im} a \neq 0$. For complex a's, the function $\sqrt{a}$ is understood as $\sqrt{a} = \sqrt{|a|}e^{i\varphi/2}$, where $\varphi \in [-\pi/2,\,\pi/2]$ is the phase of a. With this formula we find the answer:

$$u(x,t) \;=\; \frac{c}{2\sqrt{\pi t}}\, e^{-x^2/4t} \;. \tag{32}$$

It is instructive to physically analyze the answer. We see that we are dealing with a spatially localized profile of the function u, centered at the point $x = 0$. [We can also re-center the profile at any given point x_0 by the transformation $x \rightarrow x - x_0$. Note that this transformation implies $g_k \rightarrow e^{-ikx_0} g_k$.] The profile gets wider with time, an the typical width—that can be found from the requirement that the exponent is on the order one—is proportional to $\sqrt{t}$. The amplitude of the profile decreases in such a way that the integral

$$\int_{-\infty}^{\infty} u(x,t)\, dx \;=\; g(k=0,t) \;=\; c \tag{33}$$

remains constant, which is a general property of *any* localized solution of the heat equation on the infinite axis, because

$$\frac{\partial}{\partial t}\int_{-\infty}^{\infty} u(x,t)\, dx \;=\; \int_{-\infty}^{\infty} u_t(x,t)\, dx \;=$$
$$\int_{-\infty}^{\infty} u_{xx}(x,t)\, dx \;=\; u_x(\infty,t) - u_x(-\infty,t) \;=\; 0 \;. \tag{34}$$

The solution (32) features a property known as *self-similarity*: it preserves its spatial shape, up to re-scaling the coordinate x and the amplitude of u.

It is remarkable that the above qualitative physical analysis can be done without explicitly performing the integral (30). The trick is to properly re-scale (non-dimensionalize) the integration variable. Non-dimensionalizing the integration variable is a simple and powerful tool of qualitative analysis of physical answers, especially when the integrals cannot be done analytically. That is why we pay a special attention to it here, despite the fact that the answer is already known to us.

In the integral (30), instead of dimensional variable k we introduce a new dimensionless variable y such that

$$k^2 t = y^2 , \qquad (35)$$

and

$$u(x,t) = \frac{c}{2\pi\sqrt{t}} \int_{-\infty}^{\infty} dy \; e^{-y^2 + iy(x/\sqrt{t})} . \qquad (36)$$

Now we easily see that

$$u(x,t) = \frac{c}{2\pi\sqrt{t}} f(x/\sqrt{t}) , \qquad (37)$$

where

$$f(x) = \int_{-\infty}^{\infty} dy \; e^{-y^2 + iyx} \qquad (38)$$

is some function that decays at $x \to \pm\infty$. And that is all we need for establishing the above-mentioned properties, including the self-similarity.

In fact, the solution (32) is really important because *any* spatially localized solution of the heat equation asymptotically approaches Eq. (32) with the constant c given by (33). This fundamental fact is readily seen from the general solution (29). Indeed, the larger the t, the smaller the characteristic k's that contribute to the integral, because these k's are limited by the scale $1/\sqrt{t}$ at which the exponential $e^{-k^2 t}$ starts to severely decay. Each spatially localized initial Fourier transform $g(k,0)$ is characterized by its typical $k \sim k_* \sim 1/l_*$ where l_* is nothing but the inverse localization radius. Hence, at times $t \gg l_*^2$, the characteristic k in the integral is much smaller than k_*, which means that to an excellent approximation we can replace the function $q(k,0)$ with $g(0,0) = c$, and pull it out from the integral. Note that we not only proved that any localized solution approaches Eq. (32), but also estimated the characteristic time *when* it happens.

Problem 24. Suppose that the solution $u(x,t)$ of some linear PDE, obtained by the Fourier integral technique, comes in the form:

$$u(x,t) = c \int_{-\infty}^{\infty} e^{-k^4 t^7} e^{ikx} \frac{dk}{2\pi} , \qquad (39)$$

where c is a constant.

(a) Use the fast-oscillating sine/cosine ($e^{ikx} = \cos kx + i \sin kx$) argument to show that at any fixed time moment, $u(x,t) \to 0$ at $x \to \pm\infty$.

(b) Use the non-dimensionalizing trick to show that: (i) The amplitude of the solution decreases with time by the law $\propto t^{-7/4}$, (ii) the characteristic spatial width of the function $u(x,t)$ increases with time by the law $\propto t^{7/4}$, (iii) the integral $\int_{-\infty}^{\infty} u(x,t)\,dx$ is time-independent.

(c) Use the uniqueness of the Fourier-integral representation of a function to show that

$$\int_{-\infty}^{\infty} u(x,t)\,dx \;=\; c \,. \tag{40}$$

Hint/reminder: $e^{-i0x} \;=\; 1$.

Let us now consider *Schrödinger equation*

$$i\psi_t \;=\; -\psi_{xx} \,, \qquad\qquad x \in (-\infty,\,\infty)\,, \tag{41}$$

with some initial condition $\psi(x,0)$. We look for the solution in the form of the Fourier integral

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, g(k,t)\, e^{ikx} \,. \tag{42}$$

Plugging this into Eq. (41) we get

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi}\, [i\dot{g} - k^2 g]\, e^{ikx} \;=\; 0 \,, \tag{43}$$

and by uniqueness of the Fourier integral conclude that

$$i\dot{g} - k^2 g \;=\; 0 \,. \tag{44}$$

This equation is readily solved:

$$g(k,t) \;=\; g(k,0)\, e^{-ik^2 t} \,, \tag{45}$$

the initial condition $g(k,0)$ being found by Fourier transforming the function $\psi(x,0)$:

$$g(k,0) = \int_{-\infty}^{\infty} dx\, \psi(x,0)\, e^{-ikx} \,. \tag{46}$$

We thus get

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, g(k,0)\, e^{-ik^2 t + ikx} \,. \tag{47}$$

Formally, the expression looks quite similar to what we got for the heat equation. However, the number i in front of k^2 in the exponent really makes the difference. For example, the solution with $g(k,0) = \text{const}$ is of very limited physical interest since corresponding function $\psi(x,0)$ is not spatially localized.

As an important example of spatially localized initial condition, consider the Gaussian

$$\psi(x,0) = e^{-(x/l_0)^2} \ . \tag{48}$$

The function is centered at the point $x = 0$ with a characteristic width l_0. Fourier transforming this function—use Eq. (31) for doing the integral—we get

$$g(k,0) = l_0\sqrt{\pi}\, e^{-(kl_0)^2/4} \ , \tag{49}$$

and—utilizing Eq. (31) once again—find

$$\psi(x,t) = (1 + 4it/l_0^2)^{-1/2}\, e^{-\frac{x^2}{l_0^2 + 4it}} \ . \tag{50}$$

In Quantum Mechanics, the wavefunction $\psi(x)$ is not directly observable. The observable quantity is $|\psi(x)|^2$, which is interpreted as the probability density for finding the particle at the position x. Hence, keeping in mind the physics applications, we analyze the evolution of

$$|\psi(x,t)|^2 = \psi^*(x,t)\,\psi(x,t) = (1 + 16t^2/l_0^4)^{-1/2}\, e^{-\frac{2x^2 l_0^2}{l_0^4 + 16t^2}} \ . \tag{51}$$

Here the new exponent is obtained by summing up the exponent of Eq. (50) with its complex conjugate:

$$\frac{1}{l_0^2 + 4it} + \frac{1}{l_0^2 - 4it} = \frac{2l_0^2}{l_0^4 + 16t^2} \ . \tag{52}$$

Looking at Eq. (51), we see that there are two characteristic regimes: (i) small times, when $t/l_0^2 \ll 1$, and (ii) large times, when $t/l_0^2 \gg 1$. At small times, we can Taylor-expand the amplitude and the exponential in terms of the small parameter t/l_0^2, while at large times we can Taylor-expand in terms of the the small parameter l_0^2/t. Leaving only the leading terms, we get

$$|\psi(x,t)|^2 \approx e^{-2x^2/l_0^2} \qquad\qquad (t \ll l_0^2) \ , \tag{53}$$

$$|\psi(x,t)|^2 \approx (l_0^2/4t)\, e^{-x^2 l_0^2/8t^2} \qquad\qquad (t \gg l_0^2) \ . \tag{54}$$

We see that at $t \ll l_0^2$ there is basically no evolution, while at $t \gg l_0^2$ the probability distribution $|\psi(x,t)|^2$ *expands* with time, the typical width of the distribution, l_*, being directly proportional to time:

$$l_*(t) \sim t/l_0 \qquad (t \gg l_0^2) \, . \qquad (55)$$

From Eq. (54), it can be easily seen (by non-dimensionalizing the integral) that the quantity

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 \, dx \qquad (56)$$

remains constant in time. Actually, this is a general property of the solutions of Schrödinger equation that can be readily proved (to get an equation for ψ_t^*, we simply complex-conjugate the original Schrödinger equation):

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} |\psi|^2 \, dx \; = \; \int_{-\infty}^{\infty} [\psi^* \psi_t + \psi_t^* \psi] \, dx \; = \; i \int_{-\infty}^{\infty} [\psi^* \psi_{xx} - \psi_{xx}^* \psi] \, dx \; = \; 0 \, . \qquad (57)$$

Here we used

$$\int_{-\infty}^{\infty} \psi^* \psi_{xx} \, dx \; = \; \int_{-\infty}^{\infty} \psi_{xx}^* \psi \, dx \, , \qquad (58)$$

which is true because ψ is supposed to vanish at $x \to \pm\infty$, so that no boundary terms appear when doing the integrals by parts.

Now we want to explore the asymptotic behavior (at large t) of the solution with an arbitrary initial state $\psi(x,0)$. To this end we note that at large enough t (namely, $t \gg l_0^2$, where l_0 is the typical width of the initial state) the exponential e^{-ik^2t+ikx} in Eq. (47) has a rapidly changing— as a function of k—phase, $\Phi(k) = -k^2t + kx$. This means that the real and imaginary parts of the exponential are rapidly oscillating functions that effectively nullify the integrand everywhere except for a small vicinity of the so-called stationary-phase point k_0, defined by the condition

$$\Phi'(k_0) = 0 \qquad \Rightarrow \qquad k_0 = \frac{x}{2t} \, . \qquad (59)$$

And this leads to an important simplification: The function $g(k,0)$ in the integral (47) can be safely replaced with $g(k_0,0)$, and then pulled out. What remains is the Gaussian integral which is done by the formula (31) with the result

$$\psi(x,t) \; = \; \frac{e^{-i\pi/4} \, e^{ix^2/4t}}{2\sqrt{\pi t}} \; g(k = x/2t, \, 0) \qquad (t \gg l_0^2) \, . \qquad (60)$$

For $|\psi|^2$, which is the quantity of our prime physical interest, we have:

$$|\psi(x,t)|^2 \; = \; \frac{1}{4\pi t} \, |g(k = x/2t, \, 0)|^2 \qquad (t \gg l_0^2) \, . \tag{61}$$

Our result says that at $t \gg l_0^2$ there is a strict relation between the space-time position (x,t) and the wavevector k defining the value of the function $\psi(x,t)$. It turns out that for a given (x,t) only $k = x/2t$ is relevant! To put it different, at $t \gg l_0^2$, the contribution from given wavevector k propagates in space-time with a fixed velocity $v(k) = 2k$, and does not interfere with contributions from other k's. [Note that this picture *does not* take place at smaller times !] It is also worth noting that for $x = 0$ Eq. (61) yields:

$$|\psi(0,t)|^2 \; = \; \frac{1}{4\pi t} \, |g(0, \, 0)|^2 \qquad (t \gg l_0^2) \, , \tag{62}$$

from which it is directly seen that $|\psi(0,t)|^2$ decreases with time as $1/t$, and which implies—given the conservation of $\int |\psi|^2 dx$—that the width of distribution increases linearly with time.

Problem 25. Use the Fourier-integral technique to solve the wave equation

$$u_{tt} \; = \; c^2 u_{xx} \, , \qquad x \in (-\infty, \, \infty) \tag{63}$$

with the initial conditions

$$u(x,0) \; = \; e^{-(x/l_0)^2} \, , \qquad u_t(x,0) \; = \; 0 \, . \tag{64}$$

Most important part (!) Analyze the answer obtained and describe in words what is going on with the function $u(x,t)$ with increasing the time, and especially when t becomes much larger than l_0/c.

Technical comment. When restoring the solution of the wave equation from its Fourier transform, one normally has to do the integrals

$$\int_{-\infty}^{\infty} \sin(k\lambda) \, e^{(\dots)} \, dk \, , \qquad \int_{-\infty}^{\infty} \cos(k\lambda) \, e^{(\dots)} \, dk \, , \tag{65}$$

where $e^{(\dots)}$ is a Gaussian of k, and λ is some parameter. The standard exponential representation for sines and cosines,

$$\cos(k\lambda) \; = \; \frac{e^{ik\lambda} + e^{-ik\lambda}}{2} \, , \qquad \sin(k\lambda) \; = \; \frac{e^{ik\lambda} - e^{-ik\lambda}}{2i} \, , \tag{66}$$

immediately reduces each of these integrals to just a sum of two Gaussian integrals, each of which can be then done by Eq. (31).