Fourier Theory

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Abstract

In this article, we discuss the applications of complex analysis in Fourier theory results and their applications in quantum mechanics. Specifically, we derive the Fourier inversion formula and the Poisson summation formula using contour integration, and then apply these results to wave-function transformations and the free-particle Schrödinger equation.

1 Analysis Preliminaries

Definition 1.1 (Schwartz function)**.** A function $f\colon \mathbb{R} \to \mathbb{C}$ is called a Schwartz function if for every $c \in \mathbb{R}$ and every $n \in \mathbb{N}_0$,

$$\left|f^{(n)}(x)\right| = o\big(|x|^{-c}\big) \quad \text{as } |x| \to \infty.$$

Hence, f and all its derivatives decay faster than any power of $1/|x|$ at infinity.

Definition 1.2 (Fourier Exponential Series)**.** A function f is called an L periodic complex valued function if it has an expansion

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \, e^{i \frac{2\pi n}{L} x},$$

where the Fourier coefficients are

$$c_n = \frac{1}{L} \int_{-L/2}^{L/2} f(x) \, e^{-i \frac{2\pi n}{L} x} \, dx.$$

Definition 1.3 (The classes F_a and F)**.** Fix $a > 0$ and set

$$S_a \;:=\; \big\{\, z \in \mathbb{C} : |\Im z| < a \,\big\},$$

the horizontal strip of half height a. We define F_a to be the collection of functions $f\colon \mathbb{R} \to \mathbb{C}$ that extend to a holomorphic function on the strip S_a and such that there exists a constant $A > 0$ such that

$$|f(x+iy)| \;\le\; \frac{A}{1+x^2}, \qquad \text{for all } x \in \mathbb{R} \text{ and } |y| < a.$$

Finally we set the class of all functions that belong to some F_a as

$$F \;:=\; \bigcup_{a>0} F_a,$$

Definition 1.4 ($L^1(\mathbb{R})$)**.** A measurable function $f\colon \mathbb{R} \to \mathbb{C}$ is in the $L^1(\mathbb{R})$ space if

$$\|f\|_1 := \int_{\mathbb{R}} |f(x)|\, dx \;<\; \infty.$$

This means that f is absolutely integrable or that the total area under $|f|$ is finite in the space.

Theorem 1.1 (Fubini's Theorem)**.** *Let $f(x, y)$ be continuous on the rectangle*

$$R = [a, b] \times [c, d].$$

Then

$$\iint_R f(x, y)\, dA = \int_c^d \Big(\int_a^b f(x, y)\, dx\Big)\, dy = \int_a^b \Big(\int_c^d f(x, y)\, dy\Big)\, dx.$$

2 Fourier Transforms and the Fourier Inversion Theorem

Fourier Transform is a result in mathematics that takes a function as input and then outputs another function that describes the extent to which various frequencies are present in the original function. We begin by showing how to derive a Fourier transform from the series.

A length-L periodic function can only contain exponential waves whose wavelengths divide L, so its Fourier expansion is a discrete sum with coefficients c_n. If we now let $L \to \infty$, the function becomes effectively aperiodic. This means that the wavenumbers $k_n = n/L$ pack closer and closer together until they fill the real line, and the discrete list c_n is replaced by a continuous amplitude function $\hat{f}(k)$.

Periodic functions possess a discrete set of Fourier frequencies, whereas aperiodic functions possess a continuous set. We work in the Schwartz space $\mathcal{S}(\mathbb{R})$ (defined by Schwartz functions), whose rapid decay and smoothness guarantee that the inner products defining the Fourier coefficients converge. A periodic function expands as the series

$$f(x) = \sum_{n\in\mathbb{Z}} c_n\, e^{2\pi i n x/L},$$

using only those exponentials whose wavelengths divide the period L, whereas an aperiodic function expands as the integral

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(k)\, e^{2\pi i k x}\, dk,$$

where the frequency variable k varies continuously. The coefficients c_n and the amplitude $\hat{f}(k)$ are recovered through an inner product just as one extracts vector coordinates along an orthonormal basis in elementary linear algebra. The properties of $\mathcal{S}(\mathbb{R})$ ensure that each of these integrals is well defined.

Now we derive the Fourier Transform. We set

$$k_n = \frac{n}{L}, \qquad \Delta k = \frac{1}{L},$$

and define

$$\tilde{f}(k_n) \;=\; L\, c_n \;=\; \int_{-L/2}^{L/2} f(x)\, e^{-2\pi i k_n x}\, dx.$$

Letting $L \to \infty$ (so that k_n becomes continuous) gives the Fourier transform

$$\hat{f}(k) \;=\; \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i k x}\, dx, \qquad k \in \mathbb{R}.$$

Remark. *We could also define the kernel as* e^{-ikx} *and compensate with prefactors* $1/\sqrt{2\pi}$ *or* $1/2\pi$*. Our choice* $e^{-2\pi i k x}$ *keeps the transform and its inverse free of any numerical factors. However, one can't use the prefactors* $1/\sqrt{2\pi}$ *or* $1/2\pi$ *and define the kernel as* $e^{-2\pi i k x}$ *at the same time. The sign in the exponent is also a matter of convention.*

The inverse of $\hat{f}$ is given by the Fourier inversion theorem, which we prove below.

Theorem 2.1 (Fourier Inversion Theorem)**.** *Assume* $f \in F_a$ *for some* $a > 0$*, and that*

$$\hat{f}(k) = \int_{-\infty}^{\infty} f(u)\, e^{-2\pi i\, u\, k}\, du \quad \text{with} \quad f,\ \hat{f} \in L^1(\mathbb{R}).$$

Then for every $x \in \mathbb{R}$*,*

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(k)\, e^{2\pi i\, x\, k}\, dk.$$

Proof. Assume $f \in F_a$ for some $a > 0$, such that $0 < b < a$. For every $R > 0$ we denote the contour we will be integrating by γ_R which is defined by a rectangle with vertices

$$-R,\ R,\ R + ib,\ -R + ib,$$

whose lower side is $L_1 = \{u - ib : u \in \mathbb{R}\}$ and upper side is $L_2 = \{u + ib : u \in \mathbb{R}\}$.

For $k > 0$ define

$$\hat{f}(k) = \int_{-\infty}^{\infty} f(u - ib)\, e^{-2\pi i (u - ib)\, k}\, du.$$

Hence,

$$\begin{aligned}\int_0^\infty \hat{f}(k)\, e^{2\pi i x k}\, dk &= \int_{-\infty}^\infty f(u-ib) \int_0^\infty e^{-2\pi i (u-ib-x)\, k}\, dk\, du \\ &= \int_{-\infty}^\infty f(u-ib)\, \frac{1}{2\pi b + 2\pi i\,(u-x)}\, du \\ &= \frac{1}{2\pi i} \int_{L_1} \frac{f(w)}{w-x}\, dw,\end{aligned}$$

where $w = u - ib$ and $L_1 = \{u - ib : u \in \mathbb{R}\}$ is traversed left to right.

Similarly, for $k < 0$, because we are traversing this side in the opposite direction,

$$\int_{-\infty}^0 \hat{f}(k)\, e^{2\pi i x k}\, dk = -\frac{1}{2\pi i} \int_{L_2} \frac{f(w)}{w-x}\, dw,$$

where $L_2 = \{u + ib : u \in \mathbb{R}\}$, also oriented left to right.

Now, for fixed $x \in \mathbb{R}$, the function $w \mapsto f(w)/(w-x)$ has a simple pole at $w = x$ with residue $f(x)$. Thus for any large rectangular contour γ_R enclosing x,

$$f(x) = \frac{1}{2\pi i} \int_{\gamma_R} \frac{f(w)}{w-x}\, dw.$$

Letting $R \to \infty$, the vertical sides have $|f(w)| \le C(1+|w|)^{-2-\varepsilon}$ while their length is $2b$, so each side's contribution is $O(R^{-1-\varepsilon}) \to 0$. Hence γ_R deforms to $L_1 - L_2$.

Therefore,

$$\begin{aligned}f(x) &= \frac{1}{2\pi i}\Big(\int_{L_1} \frac{f(w)}{w-x}\, dw - \int_{L_2} \frac{f(w)}{w-x}\, dw\Big) \\ &= \int_0^\infty \hat{f}(k)\, e^{2\pi i x k}\, dk \;+\; \int_{-\infty}^0 \hat{f}(k)\, e^{2\pi i x k}\, dk \\ &= \int_{-\infty}^\infty \hat{f}(k)\, e^{2\pi i x k}\, dk.\end{aligned}$$

□

3 Properties of the Fourier Transform

The Fourier Transform has several properties that expand on its application. Here, $\overset{\mathcal{F}}{\longleftrightarrow}$ represents a Fourier transform.

Lemma 3.1. *For any $a, b \in \mathbb{C}$ and integrable functions $f, g\colon \mathbb{R} \to \mathbb{C}$,*

$$a\, f(x) + b\, g(x) \;\overset{\mathcal{F}}{\longleftrightarrow}\; a\, \hat{f}(k) + b\, \hat{g}(k).$$

Proof. Using $\widehat{h}(k) = \int_{-\infty}^{\infty} h(x)\, e^{-2\pi i x k}\, dx$ and the linearity of the integral,

$$\widehat{af + bg}\,(k) = \int_{-\infty}^{\infty} \big(af(x) + bg(x)\big) e^{-2\pi i x k}\, dx = a\,\hat{f}(k) + b\,\hat{g}(k).$$

□

Lemma 3.2. *If* $f(x) \overset{\mathcal{F}}{\longleftrightarrow} \hat{f}(k)$*, then for any* $x_0 \in \mathbb{R}$*,*

$$f(x - x_0) \;\overset{\mathcal{F}}{\longleftrightarrow}\; e^{-2\pi i k x_0}\,\hat{f}(k).$$

Proof. Set $u = x - x_0$ in the definition:

$$\mathcal{F}\big[f(\,x - x_0)\big](k) = \int_{-\infty}^{\infty} f(u)\, e^{-2\pi i (u + x_0) k}\, du = e^{-2\pi i k x_0}\,\hat{f}(k).$$

□

Lemma 3.3. *If* $f(x) \overset{\mathcal{F}}{\longleftrightarrow} \hat{f}(k)$*, then for any* $k_0 \in \mathbb{R}$*,*

$$e^{2\pi i k_0 x}\, f(x) \;\overset{\mathcal{F}}{\longleftrightarrow}\; \hat{f}(k - k_0).$$

Proof.

$$\mathcal{F}\big[e^{2\pi i k_0\,\cdot}\, f\big](k) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x (k - k_0)}\, dx = \hat{f}(k - k_0).$$

□

Lemma 3.4. *Let* $n \in \mathbb{N}$*. If* $f, f', \ldots, f^{(n)} \in L^1(\mathbb{R})$ *(a condition automatically satisfied when* f *is in the Schwartz Space), then*

$$f^{(n)}(x) \;\overset{\mathcal{F}}{\longleftrightarrow}\; (2\pi i k)^n\, \hat{f}(k).$$

Proof. Because a Schwartz function and all of its derivatives decay faster than any power of $|x|^{-1}$, each function belongs to $L^1(\mathbb{R})$. This rapid decay forces every boundary term that comes up in integration by parts to vanish. Hence, integrating by parts n times gives

$$\mathcal{F}\big[f^{(n)}\big](k) \;=\; \int_{-\infty}^{\infty} f^{(n)}(x)\, e^{-2\pi i k x}\, dx \;=\; (2\pi i k)^n\, \hat{f}(k).$$

□

Lemma 3.5. *For* $f, g \in L^1(\mathbb{R})$ *define* $(fg)(x) = \int_{-\infty}^{\infty} f(x - y) g(y)\, dy$*. Then*

$$f \cdot g \;\overset{\mathcal{F}}{\longleftrightarrow}\; \hat{f}(k)\, \hat{g}(k).$$

Proof. Applying Fubini's theorem,

$$\mathcal{F}[fg](k) = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} f(x - y) g(y)\, dy\right] e^{-2\pi i x k}\, dx = \hat{f}(k)\, \hat{g}(k).$$

□

4 Poisson Summation Formula

The Poisson Summation Formula relates the Fourier series coefficients of the periodic summation of a function to values of the function's continuous Fourier transform. This formula has various applications which we discuss after the proof.

Theorem 4.1 (Poisson summation formula)**.** *For a smooth, complex-valued function $f(x)$ on $\mathbb{R}$ which decays at infinity with all derivatives (Schwartz function), the Poisson summation formula states that*

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \hat{f}(k).$$

where $\hat{f}$ is the Fourier transform of f.

Proof. Choose b such that $0 < b < a$ for a function in the family F_a. Let Γ_N be the contour that we will integrate over, and let it be defined by a rectangle with vertices

$$-N - \tfrac{1}{2} - ib, \quad N + \tfrac{1}{2} - ib, \quad N + \tfrac{1}{2} + ib, \quad -N - \tfrac{1}{2} + ib,$$

whose lower side is $L_1 = \{N - 1/2 - ib : N \in \mathbb{R}\}$ and upper side is $L_2 = \{N + 1/2 - ib :: N \in \mathbb{R}\}$.

Since

$$\frac{f(z)}{e^{2\pi i z} - 1}$$

has simple poles at each integer n with residue $\frac{f(n)}{2\pi i}$, the residue theorem on Γ_N gives

$$\sum_{|n| \leq N} f(n) \;=\; \frac{1}{2\pi i} \int_{\Gamma_N} \frac{f(z)}{e^{2\pi i z} - 1}\, dz.$$

As $N \to \infty$, the vertical edges each have value $O(N^{-1-\varepsilon}) \to 0$ because of the strip decay, so only the horizontal edges will contribute, giving

$$\sum_{n \in \mathbb{Z}} f(n) \;=\; \frac{1}{2\pi i} \Big(\int_{L_1} \frac{f(z)}{e^{2\pi i z} - 1}\, dz \;-\; \int_{L_2} \frac{f(z)}{e^{2\pi i z} - 1}\, dz \Big),$$

where L_1 is the lower horizontal line $\Im z = -b$ and L_2 is the upper one $\Im z = +b$.

On L_1, $|e^{2\pi i z}| = e^{2\pi b} > 1$, so we expand

$$\frac{1}{e^{2\pi i z} - 1} = \frac{1}{e^{2\pi i z}} \sum_{m=0}^{\infty} e^{-2\pi i m z}.$$

Therefore

$$\int_{L_1} \frac{f(z)}{e^{2\pi i z} - 1}\, dz = \sum_{m=0}^{\infty} \int_{L_1} f(z)\, e^{-2\pi i (m+1) z}\, dz,$$

Since, each of these integrals can be shifted down to the real axis,

$$\int_{-\infty}^{\infty} f(x)e^{-2\pi i(m+1)x}\,dx = \hat{f}(m+1).$$

Hence

$$\int_{L_1} \frac{f(z)}{e^{2\pi iz}-1}\,dz = \sum_{m=0}^{\infty} \hat{f}(m+1).$$

On L_2, $|e^{2\pi iz}| = e^{-2\pi b} < 1$, so we use

$$\frac{1}{e^{2\pi iz}-1} = -\sum_{m=0}^{\infty} e^{2\pi imz},$$

which leads to

$$-\int_{L_2} \frac{f(z)}{e^{2\pi iz}-1}\,dz = \sum_{m=0}^{\infty}\int_{L_2} f(z)\,e^{2\pi imz}\,dz = \sum_{m=0}^{\infty} \hat{f}(-m).$$

Putting it all together,

$$\sum_{n\in\mathbb{Z}} f(n) = \sum_{m=0}^{\infty} \hat{f}(m+1) + \sum_{m=0}^{\infty} \hat{f}(-m) = \sum_{k\in\mathbb{Z}} \hat{f}(k),$$

□

The Poisson summation formula has many applications in number theory, heat kernel, and analysis. For example, we can derive the "functional equation" of the theta function using this formula.

Lemma 4.2. *For $\Re(s) > 0$, define*

$$\theta(s) \;=\; \sum_{n=-\infty}^{\infty} e^{-\pi n^2 s}.$$

Then

$$\theta(s) \;=\; s^{-1/2}\,\theta\big(1/s\big).$$

Proof. Let $f(x) = e^{-\pi s x^2}$. Its Fourier transform is

$$\hat{f}(p) = \int_{-\infty}^{\infty} e^{-\pi s x^2} e^{-2\pi i x p}\,dx = \frac{1}{\sqrt{s}}\,e^{-\pi p^2/s}.$$

By the Poisson summation formula,

$$\sum_{n\in\mathbb{Z}} e^{-\pi s n^2} = \sum_{n\in\mathbb{Z}} \hat{f}(n) = \frac{1}{\sqrt{s}} \sum_{n\in\mathbb{Z}} e^{-\pi n^2/s},$$

from which $\theta(s) = s^{-1/2}\,\theta(1/s)$.

□

5 Applications of Fourier Theory in Quantum Mechanics

5.1 Position and Momentum Space Representations

An application of the Fourier Transform is in the field of Quantum Mechanics. The Fourier Transform allows physicists to precisely model equations in quantum mechanics in a mathematical context. In quantum mechanics, a particle's state of motion is defined by $\psi(x)$, a complex valued function called the wavefunction. This function describes the mathematical description of the likelihood of finding the particle at various positions in space. The Fourier function $\widehat{\psi}(p)$ of the wave function $\psi(x)$ describes the probability amplitude of the particle's momentum space. The formulas are defined as

$$\widehat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx,$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}(p)\, e^{ipx/\hbar}\, dp.$$

where $\psi(x)$ is the Fourier transform of $\widehat{\psi}(p)$.

Here, notice that using the Fourier transform, we can switch between the momentum and position of a particle, and that one can be used to find the other.

Remark. *The $1/\sqrt{2\pi}$ factor matches the 2π scaled convention used in the previous sections.*

5.2 The Free–Particle Schrödinger Equation

The Schrödinger equation plays the role of Newton's laws and conservation of energy in classical mechanics at a quantum level. It is a wave equation in terms of the wavefunction that analytically predicts the probability of outcomes, such as where a particle is. The state of a particle moving on the line is described by a wavefunction $\psi(x,t) \in \mathbb{C}$. When the particle is free of external forces, the wavefunction must satisfy the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t}(x,t) \;=\; -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}(x,t), \qquad -\infty < x < \infty,\ t \geq 0,$$

where $\hbar$ is Planck's constant and $m > 0$ is the particle's mass.

The equation is linear with constant coefficients, so Fourier analysis allows us to derive a solution for this equation. Throughout this section, we assume the initial data ψ_0 is a Schwartz function, where $\psi_0(x) = \psi(x,0)$.

Theorem 5.1 (Free-particle solution)**.** *For every $t \geq 0$, the unique solution to the one-dimensional free Schrödinger equation*

$$i\hbar \frac{\partial \psi}{\partial t}(x,t) \;=\; -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}(x,t), \qquad \psi(x,0) = \psi_0(x),$$

is

$$\psi(x,t) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}_0(k)\, \exp\Big[i\,\frac{kx}{\hbar} - i\,\frac{\hbar k^2}{2m}\,t\Big]\, dk,$$

where

$$\widehat{\psi}_0(k) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi_0(y)\, e^{-\,iky/\hbar}\, dy$$

is the Fourier transform of the initial state. Hence, $\widehat{\psi}_0(k)$ is the momentum-space amplitude at $t = 0$, and the integral above is its inverse Fourier transform multiplied by the free particle phase factor $e^{-i\hbar k^2 t/2m}$.

Proof. For each fixed $t \geq 0$, define the Fourier transform of the function by

$$\widehat{\psi}(k,t) := \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x,t)\, e^{-\,ikx/\hbar}\, dx.$$

Now we apply the properties of the Fourier Transform to the ψ function. Because $\psi(x,t)$ and all its x-derivatives decay rapidly as $|x| \to \infty$, we differentiate under the integral sign and integrate by parts without boundary terms.

$$\mathcal{F}_x\big[\partial_t \psi(\cdot,t)\big](k) = \frac{\partial}{\partial t}\,\widehat{\psi}(k,t), \quad \mathcal{F}_x\big[\partial_x^2 \psi(\cdot,t)\big](k) = -\frac{k^2}{\hbar^2}\,\widehat{\psi}(k,t).$$

Applying the Fourier transform (in x) to the free-particle Schrödinger equation

$$i\hbar\,\partial_t \psi(x,t) = -\frac{\hbar^2}{2m}\,\partial_x^2 \psi(x,t)$$

gives for each k,

$$i\hbar\,\frac{\partial\widehat{\psi}}{\partial t}(k,t) = \frac{\hbar^2 k^2}{2m}\,\widehat{\psi}(k,t).$$

This ordinary differential equation in t has the solution

$$\widehat{\psi}(k,t) = \widehat{\psi}(k,0)\,\exp\Big(-i\,\frac{\hbar k^2}{2m}\,t\Big),$$

where $\widehat{\psi}(k,0)$ is the Fourier transform of the initial wave-function $\psi(x,0)$.

Finally, inverting the transform,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}(k,t)\, e^{\,ikx/\hbar}\, dk = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}(k,0)\, e^{-\,i\hbar k^2 t/(2m)} e^{\,ikx/\hbar}\, dk.$$

Absolute convergence of each integral follows from the rapid decay of ψ and its derivatives, which ensures that $\widehat{\psi}(k,0)$ decays faster than any power of $|k|$. Hence, differentiation under the integral sign is justified.

□

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