Fourier Series and 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 $\{e_n(x)\}$, $n = 1, 2, 3, \ldots$ 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

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

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

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

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

where

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

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

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

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 may consider (7) as an integral sum corresponding to a continuous variable n. That is in the limit of $L \to \infty$ we can replace the summation over discrete n with the integration over continuous n. Finally, introducing the new continuous variable $k = 2\pi n/L$, we arrive at (14)-(15).

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

$$f_{-k} = f_k^* \; , \tag{16}$$

by complex-conjugating Eq. (14).

Application to Green's function problem

Fourier transform is the most powerful tool for finding Green's functions of linear PDE's in the cases with translational invariance. Below we illustrate this by two simple (and closely related) examples: 1D heat equation and 1D Schrödinger equation. A detailed discussion of the application of the Fourier transform technique to the Green's function problem will be given in a separate section.

Previously, we have found that the Green's function of the 1D heat equation satisfies the relations

$$\gamma G_t = G_{xx} \; , \tag{17}$$

$$\lim_{t\to 0} \int G(x,t)\, \tilde{q}(x)\, dx \; = \; \tilde{q}(0) \; , \qquad\qquad \forall\, \tilde{q}(x) \; . \tag{18}$$

We introduce a new function, $g(k,t)$, as the Fourier transform of $G(x,t)$ with respect to the variable x, the variable t playing the role of a parameter:

$$G(x,t) = \int \frac{dk}{2\pi}\, \mathrm{e}^{ikx} g(k,t) \; . \tag{19}$$

We then plug it into (17), perform differentiation under the sign of integral, which, in particular, yields

$$G_{xx}(x,t) = -\int \frac{dk}{2\pi}\, k^2\, \mathrm{e}^{ikx} g(k,t) \; , \tag{20}$$

and get

$$\int \frac{dk}{2\pi}\, \mathrm{e}^{ikx}\, [\gamma g_t + k^2\, g] = 0 \; . \tag{21}$$

By the uniqueness of the Fourier transform we conclude that

$$\gamma g_t + k^2 \, g = 0 \; . \tag{22}$$

We have reduced a PDE problem for $G(x,t)$ to an ordinary differential equation for $g(k,t)$. The initial condition $g(k,t=0)$ is readily found from (18). By definition,

$$g(k,t) = \int dx \, \mathrm{e}^{-ikx} \, G(x,t) \; , \tag{23}$$

and, identifying e^{-ikx} with $\tilde{q}(x)$ in (18), we get

$$g(k,0) = 1 \; . \tag{24}$$

Solving (22) with (24), we find

$$g(k,t) = \mathrm{e}^{-k^2 t/\gamma} \; . \tag{25}$$

Problem 37. Restore $G(x,t)$ from this $g(k,t)$.

Problem 38. Find $g(k,t)$ for 1D Schrödinger equation and restore $G(x,t)$.

Fourier integral in higher dimensions

The Fourier transform theory is readily generalized to $d > 1$. In 1D we introduced the Fourier integral as a limiting case of the Fourier series at $L \to \infty$. Actually, the theory can be developed without resorting to the series. In d dimensions, the Fourier transform $g(\mathbf{k})$ of the function $f(\mathbf{r})$ is defined as

$$g(\mathbf{k}) = \int \mathrm{e}^{-i\mathbf{kr}} f(\mathbf{r}) \, d\mathbf{r} \; , \tag{26}$$

where $\mathbf{k} = (k_1, k_2, \ldots, k_d)$ and $\mathbf{r} = (r_1, r_2, \ldots, r_d)$ are d-dimensional vectors, $d\mathbf{r} = \prod_{j=1}^{d} dr_j$, the integral is over the whole d-dimensional space. We use a shorthand notation for the inner product of vectors: $\mathbf{kr} \equiv \mathbf{k} \cdot \mathbf{r}$. If the integral (26) is not convergent, we may introduce an enhanced version of the Fourier transform, say

$$g(\mathbf{k}) = \lim_{\epsilon_0 \to +0} \int \mathrm{e}^{-i\mathbf{kr} - \epsilon_0 r} f(\mathbf{r}) \, d\mathbf{r} \; , \tag{27}$$

or

$$g(\mathbf{k}) = \lim_{\epsilon_0 \to +0} \int \mathrm{e}^{-i\mathbf{kr}-\epsilon_0 r^2} f(\mathbf{r})\, d\mathbf{r} \ . \tag{28}$$

[The particular form of the enhancement is a matter of convenience and thus is associated with the form of $f(\mathbf{r})$.]

Moreover, if the limit $\epsilon_0 \to +0$ is ill-defined, we may keep ϵ_0 as a finite parameter, say,

$$g_{\epsilon_0}(\mathbf{k}) = \int \mathrm{e}^{-i\mathbf{kr}-\epsilon_0 r^2} f(\mathbf{r})\, d\mathbf{r} \ . \tag{29}$$

To put it different, if the function $f(\mathbf{r})$ is not good enough for the convergence of the integral (26), we replace it with a much better function, say, $\mathrm{e}^{-\epsilon_0 r^2} f(\mathbf{r})$, keeping in mind that the two are unambiguously related to each other.

The crucial question is: How to restore $f(\mathbf{r})$ from a given $g(\mathbf{k})$? The answer comes from considering the limit

$$I(\mathbf{r}) = \lim_{\epsilon \to +0} \int \mathrm{e}^{i\mathbf{kr}-\epsilon k^2} g(\mathbf{k})\, d\mathbf{k}/(2\pi)^d \ . \tag{30}$$

Substituting the r.h.s. of (26) for $g(\mathbf{k})$ and interchanging the orders of the integrations, we get

$$I(\mathbf{r}) \ = \ \lim_{\epsilon \to +0} \int d\mathbf{r}' f(\mathbf{r}') \int \mathrm{e}^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')-\epsilon k^2}\, d\mathbf{k}/(2\pi)^d \ . \tag{31}$$

Then,

$$\int \mathrm{e}^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')-\epsilon k^2} \frac{d\mathbf{k}}{(2\pi)^d} = \prod_{j=1}^{d} \int \mathrm{e}^{ik_j(r_j-r_j')-\epsilon k_j^2} \frac{dk_j}{2\pi} \ . \tag{32}$$

Utilizing the known result

$$\int_{-\infty}^{\infty} \mathrm{e}^{-ax^2+bx}\, dx \ = \ \sqrt{\frac{\pi}{a}}\, \mathrm{e}^{b^2/4a} \ , \tag{33}$$

we obtain

$$I(\mathbf{r}) = \lim_{\epsilon \to +0} \int d\mathbf{r}' f(\mathbf{r}') \prod_{j=1}^{d} \frac{\mathrm{e}^{-(r_j-r_j')^2/\epsilon}}{\sqrt{\pi\epsilon}} \ . \tag{34}$$

We see that the structure of the exponentials guarantees that if $\epsilon \to 0$, then the contribution to the integral comes from an arbitrarily small vicinity of the point $\mathbf{r}' = \mathbf{r}$. We thus can replace $f(\mathbf{r}') \to f(\mathbf{r})$ and get

$$I(\mathbf{r}) = f(\mathbf{r}) \lim_{\epsilon \to +0} \int d\mathbf{r}' \prod_{j=1}^{d} \frac{\mathrm{e}^{-(r_j-r_j')^2/\epsilon}}{\sqrt{\pi\epsilon}} = f(\mathbf{r}) \lim_{\epsilon \to +0} \prod_{j=1}^{d} \int \frac{\mathrm{e}^{-(r_j-r_j')^2/\epsilon}}{\sqrt{\pi\epsilon}} dr_j' \ . \tag{35}$$

In the r.h.s. we have a product of d identical integrals. From (33) we see that they are ϵ-independent and equal to unity. Hence, $I(\mathbf{r}) \equiv f(\mathbf{r})$.

We thus conclude that given the Fourier transform g of the function f, we can unambiguously restore f by the formula

$$f(\mathbf{r}) = \lim_{\epsilon \to +0} \int \mathrm{e}^{i\mathbf{kr} - \epsilon k^2} g(\mathbf{k})\, d\mathbf{k}/(2\pi)^d \; . \tag{36}$$

Actually, the factor $\mathrm{e}^{-\epsilon k^2}$ and, correspondingly, taking the limit is necessary only if the integral is not well defined (as is the case in many practical applications!). It is also instructive to look at the function $\mathrm{e}^{-\epsilon k^2} g(\mathbf{k})$ as the Fourier transform of some function $f_\epsilon(\mathbf{r})$, such that $f_\epsilon(\mathbf{r}) \to f(\mathbf{r})$, as $\epsilon \to +0$. From such an interpretation of (36) we conclude that the form of the ϵ-correction is a matter of convenience, and we can also write, say,

$$f(\mathbf{r}) = \lim_{\epsilon \to +0} \int \mathrm{e}^{i\mathbf{kr} - \epsilon k} g(\mathbf{k})\, d\mathbf{k}/(2\pi)^d \; . \tag{37}$$

As in 1D case, we see a a symmetry between (26)-(29)and (36)-(37). This symmetry implies, in particular, the uniqueness of the Fourier transform in the following sense. If $f(\mathbf{r})$ is representable in the form (36), or (37), then the function $g(\mathbf{k})$ is unique. For a real function f from the uniqueness it follows that

$$g(-\mathbf{k}) = g(\mathbf{k})^* \; . \tag{38}$$

Rotational symmetry. In practice, we often deal with functions $f(\mathbf{r})$ that depend only on $r = |\mathbf{r}|$. These functions remain the same under the rotational transformation of the radius vector

$$\mathbf{r} \;\to\; \mathbf{r}' = U\mathbf{r} \; , \tag{39}$$

where U is a unitary matrix. In such cases, the angular parts of the Fourier integrals are done by one and the same generic procedure. Before we start describing the procedure, it is worth noting that if $f(\mathbf{r}) \equiv f(r)$, then $g(\mathbf{k}) \equiv g(k)$, and vice versa. This is easily seen by performing the transformation

$$\mathbf{k} \;\to\; \mathbf{k}' = U\mathbf{k} \tag{40}$$

in the Fourier integral (26) and changing the integration variable by

$$\mathbf{r} = U\mathbf{r}' \; . \tag{41}$$

By definition of the unitary matrix, $U^\dagger U = 1$, implying $|\det U| = |\det U^\dagger| = 1$, we have

$$\mathbf{r} \cdot \mathbf{k}' = (U\mathbf{r}') \cdot (U\mathbf{k}) = \mathbf{r}' \cdot (U^\dagger U\mathbf{k}) = \mathbf{r}' \cdot \mathbf{k} \ , \tag{42}$$

and

$$d\mathbf{r} \ = \ |\det U|\, d\mathbf{r}' \ = \ d\mathbf{r}' \ . \tag{43}$$

Hence,

$$\begin{aligned} g(\mathbf{k}') = \int \mathrm{e}^{-i\mathbf{k}'\mathbf{r}} f(\mathbf{r})\, d\mathbf{r} = \int \mathrm{e}^{-i\mathbf{k}\mathbf{r}'} f(U\mathbf{r}')\, |\det U|\, d\mathbf{r}' = \\ = \int \mathrm{e}^{-i\mathbf{k}\mathbf{r}'} f(\mathbf{r}')\, d\mathbf{r}' = g(\mathbf{k}) \ , \end{aligned} \tag{44}$$

and thus $g(\mathbf{k}) \equiv g(k)$. The proof that from $g(\mathbf{k}) \equiv g(k)$ it follows that $f(\mathbf{r}) \equiv f(r)$ is analogous.

Consider the integral

$$g(k) = \int \mathrm{e}^{-i\mathbf{k}\mathbf{r}} f(r)\, d\mathbf{r} \tag{45}$$

in three and two dimensions.

3D case. We have

$$\int d^3r\, (\ldots) \ = \ \int_0^\infty dr\, r^2 \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin\theta\, (\ldots) \ . \tag{46}$$

Taking the z-axis along the vector $\mathbf{k}$ and introducing the new variable

$$\chi = \sin\theta \ , \qquad\qquad \int_0^\pi d\theta \sin\theta\, (\ldots) = \int_{-1}^1 d\chi\, (\ldots) \ , \tag{47}$$

we get (the integral over φ is trivial since the function is φ-independent)

$$g(k) = \int_0^\infty dr\, r^2\, f(r) \int_{-1}^1 d\chi\, \mathrm{e}^{-ikr\chi} \ . \tag{48}$$

Doing the integral

$$\int_{-1}^1 d\chi\, \mathrm{e}^{-ikr\chi} = \left. \frac{\mathrm{e}^{-ikr\chi}}{-ikr} \right|_{\chi=-1}^{\chi=1} = \frac{2}{kr} \sin kr \ , \tag{49}$$

we ultimately have

$$g(k) = \frac{4\pi}{k} \int_0^\infty dr\, r\, f(r) \sin kr \ . \tag{50}$$

Similarly,

$$f(r) = \frac{1}{2\pi^2 r} \int_0^\infty dk\, k\, g(k) \sin kr \ . \tag{51}$$

Hence, the 3D integrals are reduced to 1D ones.

2D case. Here we have

$$\int d^2r \,(\ldots) \ = \ \int_0^\infty dr\, r \int_0^{2\pi} d\varphi \,(\ldots) \ . \tag{52}$$

Taking the x-axis along the vector $\mathbf{k}$, we get

$$\begin{aligned} g(k) &= \int_0^\infty dr\, r\, f(r) \int_0^{2\pi} d\varphi\, \mathrm{e}^{-ikr\cos\varphi} = \\ &= \int_0^\infty dr\, r\, f(r) \int_0^{2\pi} d\varphi\, \cos(kr\cos\varphi) \ . \end{aligned} \tag{53}$$

Here we take into account that by shifting the variable $\varphi \to \varphi + \pi$ and keeping the limits of integration the same (which does not effect the value of the integral due to 2π-periodicity of the integrand) we have

$$\int_0^{2\pi} d\varphi\, \sin(kr\cos\varphi) = -\int_0^{2\pi} d\varphi\, \sin(kr\cos\varphi) \ , \tag{54}$$

which means that the integral is zero. The integral over φ leads to the Bessel function:

$$\int_0^{2\pi} d\varphi\, \cos(kr\cos\varphi) \ = \ 2\pi J_0(kr) \ . \tag{55}$$

Finally,

$$g(k) = 2\pi \int_0^\infty dr\, r\, f(r) J_0(kr) \ , \tag{56}$$

and similarly,

$$f(r) = \frac{1}{2\pi} \int_0^\infty dk\, k\, g(k) J_0(kr) \ . \tag{57}$$

Hence, the 2D integrals are reduced to 1D ones, but in contrast to the 3D case a special function enters the generic expression. In view of this fact sometimes it is convenient to do the integral over r or k first.—It may then occur that the angular part of the integral can be done in terms of the elementary functions.

Example—Coulomb potential in 3D. We want to find the Fourier transform from

$$f(r) = 1/r \; . \tag{58}$$

Plugging this into (50), we get a divergent integral

$$g(k) = \frac{4\pi}{k} \int_0^\infty dr \, \sin kr \tag{59}$$

and understand that first we need to regularize the problem. We choose the regularization

$$1/r \to \mathrm{e}^{-\epsilon r}/r \; , \tag{60}$$

which is especially convenient for this case:

$$g(k) = \frac{4\pi}{k} \int_0^\infty dr \, \mathrm{e}^{-\epsilon r} \, \sin kr \; = \; \frac{4\pi}{k} \, \mathrm{Im} \int_0^\infty dr \, \mathrm{e}^{ikr - \epsilon r} \; = \; \frac{4\pi}{k^2 + \epsilon^2} \; . \tag{61}$$

Now we can set $\epsilon = 0$ and get the result

$$g(k) \; = \; \frac{4\pi}{k^2} \; . \tag{62}$$

Note that as a by-product we have obtained the Fourier transform of the screened-Coulomb potential $\mathrm{e}^{-\kappa r}/r$, where κ is called the inverse screening radius. The Fourier transform in this case is $g(k) = 4\pi/(k^2 + \kappa^2)$.

Problem 39. Use (51) to restore a 3D function $f(r)$ from its Fourier transform $g(k)$, if

(a) $g(k) = 4\pi/k^2$,
(b) $g(k) = 4\pi/(k^2 + \kappa^2)$.

Problem 40. Find the Green's function for the d-dimensional heat equation by the Fourier transform method. *Hint.* In this particular case the inverse transform is most easily done in the Cartesian coordinates.

Problem 41. The same for d-dimensional Schrödinger equation.

Fourier integral as a unitary operator

Consider the set of complex-valued functions $f(\mathbf{r})$ for which the integral (over the whole d-dimensional space of $\mathbf{r}$)

$$\int |f(\mathbf{r})|^2 \, d\mathbf{r} \tag{63}$$

is well defined. This set is a Hilbert space with the inner product defined as

$$\langle g|f\rangle = \int g^*(\mathbf{r}) f(\mathbf{r}) \, d\mathbf{r} \; . \tag{64}$$

Within this space of functions, the Fourier integral can be viewed as a linear operator, F, that transforms one vector, $|f\rangle$, into another, $|g\rangle$:

$$|g\rangle = F\,|f\rangle \; . \tag{65}$$

Let us find the operator $F^\dagger$. By definition, $\forall\, f_1, f_2$, $\langle F^\dagger f_1|f_2\rangle = \langle f_1|F|f_2\rangle$. Hence, to find $F^\dagger$ we need to analyze an explicit expression for $\langle f_1|F|f_2\rangle$. We have

$$\langle f_1|F|f_2\rangle = \int d\mathbf{k}\, d\mathbf{r}\, \mathrm{e}^{-i\mathbf{kr}} f_1^*(\mathbf{k}) f_2(\mathbf{r}) = \int d\mathbf{r} \left[\int d\mathbf{k}\, \mathrm{e}^{i\mathbf{kr}} f_1(\mathbf{k}) \right]^* f_2(\mathbf{r}) \; , \tag{66}$$

and thus

$$F^\dagger|f_1\rangle = \int d\mathbf{k}\, \mathrm{e}^{i\mathbf{kr}} f_1(\mathbf{k}) \; , \qquad \forall f_1 \; . \tag{67}$$

We see that up to a factor $1/(2\pi)^d$, the action of the operator $F^\dagger$ is equivalent to restoring an original function from its Fourier transform. That is, $\forall f$,

$$F^\dagger F|f\rangle \;=\; (2\pi)^d \, \frac{F^\dagger}{(2\pi)^d} \, F|f\rangle \;=\; (2\pi)^d \, |f\rangle \; . \tag{68}$$

This means that up to a constant factor—which is just a matter of definition—operator F is unitary:

$$F^\dagger F = (2\pi)^d \; . \tag{69}$$

An immediate consequence of this fact is the following relation, in which $g(\mathbf{k})$ is the Fourier transform of $f(\mathbf{r})$.

$$\int |g(\mathbf{k})|^2 \, d\mathbf{k} \;=\; (2\pi)^d \int |f(\mathbf{r})|^2 \, d\mathbf{r} \; . \tag{70}$$

Indeed, in the vector notation we have

$$\langle g|g\rangle \;=\; \langle Ff|Ff\rangle \;=\; \langle F^{\dagger}Ff|f\rangle \;=\; (2\pi)^d \,\langle f|f\rangle \;. \tag{71}$$

Generalized functions and their Fourier transforms

The Green's function technique for solving translational invariant PDE's implies existence of the function $G(x,t)$, such that the solution $u(x,t)$—for the sake of definiteness, we discuss a one-dimensional time-evolution problem—is related to the initial condition, $u(x,0)$, by

$$u(x,t) = \int G(x-x_0,t)\, u(x_0,0)\, dx_0 \;. \tag{72}$$

However, for many problems this is not the case. In particular, $G(x,0)$ is *always* ill defined, since otherwise we would have

$$\int G(x,0)\, q(x)\, dx \;= q(0) \;, \qquad\qquad \forall\, q(x) \;, \tag{73}$$

which is obviously impossible in terms of any regular function $G(x,0)$. When arriving at (72) from considering the limit of $L\to\infty$ in the Fourier-series solution of a finite-interval problem, $x\in[-L/2,L/2]$, we interchange the orders of summation over the basis vectors and integration over x_0, which is not always legitimate. Nevertheless, the structure of the solution in terms of the Fourier series allows us to make a less restrictive statement that, speaking the vector language, the solution $|u(t)\rangle$ is related to the initial condition $|u(0)\rangle$ by a certain linear operator $\hat{G}$:

$$|u(t)\rangle \;=\; \hat{G}\,|u(0)\rangle \;. \tag{74}$$

The next observation is that if we cannot represent some linear operator in the form (72), we can try—and this works in all practical cases!—to use a more general formula

$$u(x,t) = \lim_{\epsilon\to+0} \int G_\epsilon(x-x_0,t)\, u(x_0,0)\, dx_0 \;, \tag{75}$$

where ϵ is some parameter and $G_\epsilon(x-x_0,t)$ is some function of this parameter which is well defined at $\epsilon>0$. And now we can use the Fourier transform technique to find $g_\epsilon(k)$, the Fourier transform of $G_\epsilon(x)$, and then restore $G_\epsilon(x)$. It is important that in contrast to the ill-defined limit

$$\lim_{\epsilon\to+0} G_\epsilon(x) \ , \tag{76}$$

normally there exists the limit

$$g(k) \ = \ \lim_{\epsilon\to+0} g_\epsilon(k) \tag{77}$$

and when solving the problem we can actually look for $g(k)$. Having found $g(k)$, we then need to introduce $g_\epsilon(k)$, because the inverse transform from $g(k)$ is supposed to be divergent—otherwise a regular function $G(x)$ would exist. The replacement $g(k) \to g_\epsilon(k)$, called *regularization*, is *arbitrary*, provided the Fourier transform from $g_\epsilon(k)$ converges. The nature of this arbitrariness is due to the fact that we are interested only in the limiting value of the integral in the r.h.s. of (75).

Example 1. Consider the simplest case $g(k) \equiv 1$. To obtain corresponding $G_\epsilon(x)$, we need to introduce a regularization. Let us try three different regularizations:

$$\begin{array}{lrcl}
\text{(a)} & g_\epsilon(k) & = & 1\cdot \mathrm{e}^{-\epsilon|k|} \ , \\
\text{(b)} & g_\epsilon(k) & = & 1\cdot \mathrm{e}^{-\epsilon k^2} \ , \\
\text{(c)} & g_\epsilon(k) & = & 1\cdot \mathrm{e}^{i\epsilon k^2} \ .
\end{array}$$

All the integrals are readily done (in the first case we integrate separately over $k<0$ and $k>0$), and the results are:

$$\begin{array}{lrcl}
\text{(a)} & G_\epsilon(x) & = & \dfrac{1}{\pi}\,\dfrac{\epsilon}{x^2+\epsilon^2} \ , \\
\text{(b)} & G_\epsilon(x) & = & \dfrac{\mathrm{e}^{-x^2/4\epsilon}}{\sqrt{4\pi\varepsilon}} \ = \ \dfrac{\mathrm{e}^{-x^2/\epsilon_0}}{\sqrt{\pi\varepsilon_0}} \qquad (\varepsilon_0 = 4\epsilon) \ , \\
\text{(c)} & G_\epsilon(x) & = & \dfrac{\mathrm{e}^{ix^2/4\epsilon}}{\sqrt{-4i\pi\varepsilon}} \ = \ \dfrac{\mathrm{e}^{ix^2/\epsilon_0}}{\sqrt{-i\pi\varepsilon_0}} \qquad (\varepsilon_0 = 4\epsilon) \ .
\end{array}$$

Considering the integral

$$\int G_\epsilon(x-x_0)\, f(x_0)\, dx_0 \ , \tag{78}$$

where f is some fixed continuous function an ϵ is *arbitrarily* small—since ultimately we are interested in the limit $\epsilon \to 0$—we notice that we can replace $q(x_0)$ with $q(x)$ and pull it out from the integral. Indeed, for all the three functions the contribution to the integral comes from a small region around the point $x_0 = x$. In the cases (a) and (b) this happens because the function $G_\epsilon(x)$ rapidly vanishes away from $x = 0$, while in the case (c) it is strongly oscillating which is equivalent to vanishing in the integral sense. Finally, we note that in all the three cases

$$\int G_\epsilon(x)\, dx \;\equiv\; g_\epsilon(k=0) \;=\; 1 \;, \tag{79}$$

and get

$$\lim_{\epsilon\to+0} \int G_\epsilon(x - x_0)\, f(x_0)\, dx_0 \;=\; f(x) \;, \qquad\qquad \forall\, f(x) \;. \tag{80}$$

Hence, the operator $\hat{G}$ that corresponds to this limiting procedure is just the unity operator:

$$\hat{G}\,|f\rangle \;=\; |f\rangle \;. \tag{81}$$

Example 2. Consider $\tilde{g}(k) = ik$. Note that whatever the regularization $\tilde{g}_\epsilon(k)$ is taken, we always have

$$\tilde{G}_\epsilon(x) \;=\; \int \frac{dk}{2\pi}\, \mathrm{e}^{ikx}\, \tilde{g}_\epsilon(k) \;=\; \int \frac{dk}{2\pi}\, \mathrm{e}^{ikx}\, ik\, g_\epsilon(k) \;, \tag{82}$$

where $g_\epsilon(k) = \tilde{g}_\epsilon(k)/ik$ is a certain regularization of the function $g(k) \equiv 1$. This allows us to reduce the problem to that of the Example 1, because

$$\tilde{G}_\epsilon(x) \;=\; \int \frac{dk}{2\pi}\, \mathrm{e}^{ikx}\, ik\, g_\epsilon(k) \;=\; \frac{d}{dx} \int \frac{dk}{2\pi}\, \mathrm{e}^{ikx}\, g_\epsilon(k) \;=\; G'_\epsilon(x) \;. \tag{83}$$

Hence,

$$\lim_{\epsilon\to+0} \int \tilde{G}_\epsilon(x - x_0)\, f(x_0)\, dx_0 \;=\; \lim_{\epsilon\to+0} \int G'_\epsilon(x - x_0)\, f(x_0)\, dx_0 \;=\; f'(x) \;, \tag{84}$$

and we see that the operator $\hat{G}$ in this case is the differential operator:

$$\hat{G}\,|f\rangle \;=\; |f'\rangle \;, \qquad\qquad f'(x) \;\equiv\; \frac{df(x)}{dx} \;. \tag{85}$$

Actually, it is very convenient to treat the ill-defined limit (76) as a *generalized function* in the following sense. A generalized function, say,

$$\Lambda(x) \;=\; \lim_{\epsilon\to+0} G_\epsilon(x)\;, \tag{86}$$

is meaningful only if it is a part of an integral over x. And its precise meaning is:

$$\int \Lambda(x)\, f(x)\, dx \;=\; \lim_{\epsilon\to+0} \int G_\epsilon(x)\, f(x)\, dx\;. \tag{87}$$

For example, the generalized function corresponding to the unity operator is known as Dirac *delta-function*, $\delta(x-x_0)$. In accordance with the results of the Example 1, the delta-function can be *represented* as

$$\delta(x) \;=\; \lim_{\epsilon\to+0} \frac{1}{\pi}\,\frac{\epsilon}{x^2+\epsilon^2} \;=\; \lim_{\epsilon\to+0} \frac{\mathrm{e}^{-x^2/\epsilon}}{\sqrt{\pi\varepsilon}} \;=\; \lim_{\epsilon\to+0} \frac{\mathrm{e}^{ix^2/\epsilon}}{\sqrt{-i\pi\varepsilon}}\;. \tag{88}$$

Then,

$$\int \delta(x-x_0)\, f(x_0)\, dx_0 \;=\; f(x)\;. \tag{89}$$

Defining the derivative $\Lambda'(x)$ of a generalized function $\Lambda(x)$ as

$$\Lambda'(x) \;=\; \lim_{\epsilon\to+0} G'_\epsilon(x)\;, \tag{90}$$

we get (doing the integral by parts)

$$\int \Lambda'(x)\, f(x)\, dx \;=\; -\lim_{\epsilon\to+0} \int G_\epsilon(x)\, f'(x)\, dx\;. \tag{91}$$

We conclude that with our definitions the generalized functions behave the same way as the ordinary functions. This proves to be very convenient for various manipulations with integrals (like differentiating with respect to a parameter or integrating by parts). The concept of the generalized function also allows us not to write explicitly the limiting expressions. For example, in accordance with the results of the Example 1, we may write

$$\int \mathrm{e}^{ikx}\, dk/2\pi \;=\; \delta(x)\;. \tag{92}$$

The precise meaning of this expression is as follows. If during some manipulations with the integrals (interchanging variables) we get the l.h.s. of Eq. (92) under the sign of integration with respect to x, then this means that the interchanging was not legitimate, but we could regularize our functions—introducing corresponding limiting procedure—in such a way that the limiting procedure leads to the delta-function. By the way, this is exactly what we did when establishing the formula for the inverse Fourier transform. From now on we can simply use (92).

The definition (90) of the generalized derivative is also good for functions with jumps.

Example 3. Consider the so-called θ-function

$$\theta(x) = \begin{cases} 1\,, & x \geq 0\,, \\ 0\,, & x < 0\,. \end{cases} \tag{93}$$

Noting that

$$\theta(x) \;=\; \lim_{\epsilon\to+0} \frac{1}{\pi} \arctan(x/\epsilon) + 1/2\,, \tag{94}$$

we find

$$\theta'(x) \;=\; \lim_{\epsilon\to+0} \frac{1}{\pi} \frac{\epsilon}{x^2+\epsilon^2} \;=\; \delta(x)\,. \tag{95}$$

Delta-function in higher dimensions. The definition of the d-dimensional δ-function, $\delta^{(d)}(\mathbf{r})$, is as follows

$$\int \delta^{(d)}(\mathbf{r}-\mathbf{r}_0)\, f(\mathbf{r}_0)\, d\mathbf{r}_0 \;=\; f(\mathbf{r})\,. \tag{96}$$

Once again $\delta^{(d)}(\mathbf{r})$ is understood as a limiting procedure. It is readily seen that $\delta^{(d)}(\mathbf{r})$ can be written in terms of one-dimensional δ-functions:

$$\delta^{(d)}(\mathbf{r}-\mathbf{r}_0) \;=\; \prod_{j=1}^{d} \delta(r_j - r_{0j})\,. \qquad \text{(Cartesian coordinates)} \tag{97}$$

$$\delta^{(2)}(\mathbf{r}-\mathbf{r}_0) \;=\; r^{-1}\,\delta(r-r_0)\,\delta(\varphi-\varphi_0)\,. \qquad \text{(Polar coordinates)} \tag{98}$$

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}_0) \;=\; \rho^{-1}\,\delta(\rho-\rho_0)\,\delta(\varphi-\varphi_0)\,\delta(z-z_0)\,. \qquad \text{(Cylindrical coord.)} \tag{99}$$

$$\delta^{(3)}(\mathbf{r}-\mathbf{r}_0) \;=\; \frac{\delta(r-r_0)\,\delta(\varphi-\varphi_0)\,\delta(\theta-\theta_0)}{r^2\sin\theta}\,. \qquad \text{(Spherical coord.)} \tag{100}$$

The d-dimensional analog of (92) immediately follows from (97):

$$\int \mathrm{e}^{i\mathbf{kr}}\, d\mathbf{k}/(2\pi)^d \;=\; \delta^{(d)}(\mathbf{r})\,. \tag{101}$$

Problem 42. The convolution, $Q(\mathbf{r})$, of two functions, $f_1(\mathbf{r})$ and $f_2(\mathbf{r})$, is defined as

$$Q(\mathbf{r}) \;=\; \int f_1(\mathbf{r}-\mathbf{r}_0)\, f_2(\mathbf{r}_0)\, d\mathbf{r}_0 \;. \tag{102}$$

[Note, that Eq. (72) is a typical example of convolution.] Use Eq. (101) to prove the formula

$$Q(\mathbf{r}) \;=\; \int \mathrm{e}^{i\mathbf{k}\mathbf{r}}\, F_1(\mathbf{k})\, F_2(\mathbf{k})\, d\mathbf{k}/(2\pi)^d \;, \tag{103}$$

where F_1 and F_2 are the Fourier transforms of the functions $f_1(\mathbf{r})$ and $f_2(\mathbf{r})$.

Problem 43. Show that if $f(x)$ is a smooth function such that

$$f(x_j) = 0 \;, \qquad\qquad j = 1, 2, \ldots, n \;, \tag{104}$$

then

$$\delta(f(x)) \;=\; \sum_{j=1}^{n} |f'(x_j)|^{-1}\, \delta(x - x_j) \;. \tag{105}$$

Problem 44. A linear operator $\hat{L}$ is represented by a generalized function $\Lambda(\mathbf{r})$:

$$\hat{L} f(\mathbf{r}) \;=\; \int \Lambda(\mathbf{r}-\mathbf{r}_0)\, f(\mathbf{r}_0)\, d\mathbf{r}_0 \;. \tag{106}$$

The Fourier transform of the generalized function $\Lambda(\mathbf{r})$ is $\lambda(\mathbf{k}) = k^2$.
Find:
(a) the generalized function $\Lambda(\mathbf{r})$
(b) the operator $\hat{L}$.