The Fourier Transform and Free Particle Wave Functions

1 The Fourier Transform

1.1 Fourier transform of a periodic function

A function $f(x)$ that is periodic with period $2L$,

$$f(x) = f(x + 2L)$$

can be expanded in a Fourier Series over the interval $(-L, L)$,

$$f(x) = \sum_{n=0}^{\infty} A_n \cos \frac{n\pi x}{L} + \sum_{n=0}^{\infty} B_n \sin \frac{n\pi x}{L}$$

Noting that the coefficients may be complex (we never said $f(x)$ was real), and recalling that $e^{i\theta} = cos\theta + i\sin\theta$, the series may be written as

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{in\pi x/L}$$

The a_n are the Fourier coefficients. Each a_n specifies the contribution to $f(x)$ of a wave $\exp(in\pi x/L)$ with wavenumber $k = n\pi/L$. The Fourier modes are orthonormal,

$$\frac{1}{2L} \int_{-L}^{L} dx \left(e^{in\pi x/L} \right)^* e^{im\pi x/L} = \frac{1}{2L} \int_{-L}^{L} dx \, e^{-in\pi x/L} e^{im\pi x/L} = \delta_{mn}$$

where δ_{mn} is the Kronecker delta function. To obtain the values of the Fourier coefficients a_n, integrate both sides of the Fourier series expansion above

$$\frac{1}{2L} \int_{-L}^{L} dx \, e^{-in\pi x/L} f(x) = \frac{1}{2L} \int_{-L}^{L} dx \, e^{-in\pi x/L} \sum_{m=-\infty}^{\infty} a_m e^{im\pi x/L}$$

and use the orthonormality of the plane waves (note that only terms with $m = n$ survive on the right hand side) to obtain the Fourier coefficients

$$a_n = \frac{1}{2L} \int_{-L}^{L} dx \, f(x) e^{-in\pi x/L}$$

1.2 Fourier integral

To proceed to the Fourier transform integral, first note that we can rewrite the Fourier series above as

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{in\pi x/L} \Delta n$$

where $\Delta n = 1$ is the spacing between successive integers. If we define

$$\Delta k = \frac{\pi \Delta n}{L}$$

and

$$A(k) = \frac{\sqrt{2\pi} L a_n}{\pi}$$

then the Fourier series may be written as

$$f(x) = \sum_{k} \frac{A(k)}{\sqrt{2\pi}} e^{in\pi x/L} \Delta k$$

Now take the limit $L \to \infty$, so that Δk becomes infinitesimal. Now the discrete sum becomes an integral,

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk$$

Following the discussion above that yielded the coefficients a_n, the coefficients $A(k)$ of the continuous transform are obtained by

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dk$$

These two equations define the Fourier transform relations. The latter is usually referred to as a *forward* transform, decomposing the spatial function $f(x)$ into Fourier modes, represented by their coefficients $A(k)$, while the former is the *inverse* transform, which reconstructs the spatial function. (Note that here I've put factors of $1/\sqrt{2\pi}$ in front of both integrals; some conventions leave out the factor in front of the forward transform and put $1/(2\pi)$ in front of the inverse transform, or vice versa.)

The functions $f(x)$ and $A(k)$ are a Fourier transform *pair*. Complete knowledge of one of the pair yields the other through an analytic transform, thus they have identical information content. They are just different representations of the same function. Note carefully that both $f(x)$ and $A(k)$ are, in general, complex. In the case where $f(x)$ is a real function, then $A(k)$ must be Hermitian, $A^*(k) = A(-k)$. The common pairs of transform spaces includes position-wavenumber and time-frequency.

1.3   Dirac Delta Function

If we combine the two equations above for $f(x)$ and $A(k)$, plugging the second into the first, we obtain

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx} \int_{-\infty}^{\infty} dy\, f(y) e^{-iky}$$

Now interchange the order of integration,

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy\, f(y) [\int_{-\infty}^{\infty} dk\, e^{ikx} e^{-iky}]$$

The term in brackets is the Dirac Delta function,

$$\delta(x - y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x-y)}$$

This function obviously has the property that

$$\int_{-\infty}^{\infty} f(y)\delta(x - y) = f(x)$$

1.4   Fourier transform pairs

If $f(x)$ is very narrow, then its Fourier transform $A(k)$ is a very broad function and vice versa. The Dirac delta function provides the most extreme example of this property. If the Fourier transform is a constant, say $A(k) = 1/\sqrt{2\pi}$, then the spatial function is exactly the function $f(x) = \delta(x)$. In this case the spatial function is precisely localized and its Fourier transform is completely delocalized. If this sounds like the uncertainty relation to you, you're on the right track.

To lead into discussion of another Fourier transform pair, let us begin with another form of the Dirac delta function. Any properly normalized (meaning that the integral over all space is unity) peaked function approaches a delta function in the limit of infinitesimal width, so a Gaussian will work,

$$\delta(x) = \lim_{\alpha \to 0} \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^x}$$

The Fourier transform of this delta function is obviously a constant function, which is the same as a Gaussian of infinite width. We can see this by considering the Fourier transform of a 1-d Gaussian

$$f(x) = \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^x}$$

which can be shown to be another Gaussian

$$A(k) = \frac{1}{\sqrt{2\pi}} e^{-k^2/(4\alpha^2)}$$

Now we clearly see the relationship between the dispersion in the spatial function and its Fourier transform. Narrowing the extent of the function in one domain broadens its extent in the other domain. For a Gaussian, the dispersions are in the relation $\sigma_x \sigma_k = 1$.

2 The Schrödinger Equation and Free Particle Wave Functions

2.1 Wave Packets

The wave-particle duality problem can be somewhat reconciled by thinking about particles as localized wave packets. Waves of different frequencies are superposed so that they interfere completely (or nearly so) outside of a small spatial region. Clearly, both the amplitudes (magnitude of waves of different frequencies) and phases (relative shifting of the waves) are required to achieve such a superposition.

A plane wave, which varies only in the x but not in y or z, has the form

$$e^{ikx-i\omega t}$$

where k is the wavenumber $k = 2\pi/\lambda$ and ω is the angular frequency of the wave. In general, $\omega = \omega(k)$. A superposition of such waves can be used to represent the wave packet

$$f(x,t) = \int_{-\infty}^{\infty} dk\, g(k) e^{ikx-i\omega(k)t}$$

If the wave packet is quite localized in $k-$space, with $g(k)$ narrowly centered at $k = k_0$, such as

$$g(k) \propto e^{-\alpha(k-k_0)^2}$$

with corresponding $\omega = \omega(k_0)$, then we can associate this wave packet with a particle that has energy

$$E = \hbar\omega$$

and momentum

$$p = \hbar k$$

This suggests that, in general, we can rewrite any wave packet as a superposition of plane waves that have a distribution of momenta p,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \phi(p) e^{i(px-Et)/\hbar}$$

2.2 Solutions to the Schrödinger equation

The wave packet $\psi(x,t)$ above is a general solution to the differential equation

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

This is the time-dependent Schrödinger equation for a free particle, i.e., where $V = 0$, written in the position representation. This shows that plane waves $\exp(ikx - i\omega t)$ are eigenfunctions of the free particle Hamiltonian.

The probability of finding a particle at position x is proportional to the squared modulus $|\psi(x,t)|^2$. Likewise, the probability of finding this same particle with momentum p is proportional to $|\phi(p)|^2$. These two representations are related by the Fourier transform relation above.

The Fourier transform relation between the position and momentum representations immediately suggests the Heisenberg uncertainty relation. We showed above that the dispersions of a spatial Gaussian and its Fourier transform are in the relation $\sigma_x \sigma_k = 1$. The product of dispersions is minimized by a Gaussian, thus in general $\Delta x \Delta k \geq 1$. Using $p = \hbar k$, this suggests that the uncertainty relation must be of order

$$\Delta x \Delta p \geq \hbar$$

3   References

More about Fourier transforms can be found in the classic text "The Fourier Transform and Its Application," R.N. Bracewell (McGraw Hill). The discussion above closely follows the development in "Quantum Physics," S. Gasiorowicz (Wiley).