The Fourier transform

When we considered a particle in a box of finite length a we stated that any "sufficiently nice" and normalizable function $\psi(x)$ can be expanded in terms of the eigenfunctions of the Hamiltonian,

$$\phi_K(x) = \sqrt{\frac{2}{a}} \sin \frac{k\pi x}{a}.$$

Essentially what that means is that we expand an arbitrary function $\psi(x)$ in the Fourier series in the interval $[-a, a]$. Since the Fourier series is a form of representing periodic functions (that go from $-\infty$ to $+\infty$) we just use this series within one half-period $[0, a]$ only, while otside this interval our function $\psi(x)$ is zero by definition.

Indeed, recall from the calculus course that any periodic function $f(x)$ integrable on an iterval $[x_0, x_0+P]$ can be approximated by a partial sum

$$f_N(x) = \frac{A_0}{2} + \sum_{n=1}^{N} A_n \sin\left(\frac{2\pi n x}{P} + \varphi_n\right) \qquad N \geq 1$$

and this partial sum converges to $f(x)$ as $N \to \infty$

Using the trigonometric identities

$$\sin\left(\frac{2\pi n x}{P} + \varphi_K\right) = \sin(\varphi_n)\cos\left(\frac{2\pi n x}{P}\right) + \cos(\varphi_n)\sin\left(\frac{2\pi n x}{P}\right)$$

and

$$\sin\left(\frac{2\pi n x}{P} + \varphi_n\right) = \mathrm{Re}\left[\frac{1}{i} e^{i\left(\frac{2\pi n x}{P} + \varphi_n\right)}\right] = \frac{1}{2i} e^{i\left(\frac{2\pi n x}{P} + \varphi_n\right)} + \left(\frac{1}{2i} e^{i\left(\frac{2\pi n x}{P} + \varphi_n\right)}\right)^*$$

we can write the above expression for $f_N(x)$ as follows:

$$f_N(x) = \frac{a_0}{2} + \sum_{n=1}^{N}\left(\underbrace{a_n}_{A_n \sin\varphi_n} \cos\left(\frac{2\pi n x}{P}\right) + \underbrace{b_n}_{A_n\cos\varphi_n} \sin\left(\frac{2\pi n x}{P}\right)\right)$$

or

$$f_N(x) = \sum_{n=-N}^{N} c_n e^{i\frac{2\pi n x}{P}} \quad \text{where} \quad c_n = \begin{cases} \frac{A_n}{2i} e^{i\varphi_n} = \frac{1}{2}(a_n - i b_n), & n>0 \\ \frac{1}{2} a_0, & n=0 \\ \frac{1}{2}(a_n + i b_n), & n<0 \end{cases}$$

and $A_n = \sqrt{a_n^2 + b_n^2}$ $\qquad \varphi_n = \arctan\left(\frac{a_n}{b_n}\right)$

The Fourier coefficients are computed using the orthogonality of cosines/sines or complex exponentials.

$$\int_{x_0}^{x_0+P} \cos\left(\frac{2\pi n x}{P}\right)\cos\left(\frac{2\pi m x}{P}\right) dx = \frac{P}{2}\delta_{nm}$$

$$\int_{x_0}^{x_0+P} \sin\left(\frac{2\pi n x}{P}\right)\cos\left(\frac{2\pi m x}{P}\right) dx = 0$$

$$\int_{x_0}^{x_0+P} \sin\left(\frac{2\pi n x}{P}\right)\sin\left(\frac{2\pi m x}{P}\right) dx = \frac{P}{2}\delta_{nm}$$

$$\int_{x_0}^{x_0+P} \left(e^{i\frac{2\pi n x}{P}}\right)^{*}\left(e^{i\frac{2\pi m x}{P}}\right) dx = P\,\delta_{nm}$$

so that

$$a_n = \frac{2}{P}\int_{x_0}^{x_0+P} f(x)\cos\left(\frac{2\pi n x}{P}\right) dx \qquad b_n = \frac{2}{P}\int_{x_0}^{x_0+P} f(x)\sin\left(\frac{2\pi n x}{P}\right) dx$$

$$c_n = \frac{1}{P}\int_{x_0}^{x_0+P} f(x)\, e^{-i\frac{2\pi n x}{P}} dx$$

Now in our case of a particle in an infinite well $(0 \le x \le a)$ we can formally set $x_0 = -a$, $P = 2a$. We also use the condition $\psi(0)=0$ (particle cannot penetrate the wall) which make all a_n vanish for any $\psi(x)$ which has this property:

Finally we get

$$b_n = \frac{1}{a}\int_{-a}^{a} f(x)\sin\frac{\pi n x}{a}\,dx$$

If we assume that $f(x)$ is odd in $[-a, a]$, which we can do because in the end we only use the Fourier series on $[0, a]$ interval, then we obtain

$$b_n = \frac{2}{a}\int_{0}^{a} f(x)\sin\frac{\pi n x}{a}\,dx$$

Also we can notice that the orthogonality condition for sin's only can be written as

$$\int_{-a}^{a}\sin\left(\frac{\pi n x}{a}\right)\sin\left(\frac{\pi m x}{a}\right)dx = a\,\delta_{nm}$$

or

$$\int_{0}^{a}\sin\left(\frac{\pi n x}{a}\right)\sin\left(\frac{\pi m x}{a}\right)dx = \frac{a}{2}\,\delta_{nm}$$

These are exactly the expressions we had for the particle in a box $(0 < x < a)$

Now let us consider the situation when the length of the box approaches infinity. That would correspond to the situation when $x_0 = -a$, $x_0 + \ell \to +a$, $\ell \to 2a$, $a \to \infty$. In this case it is more convenient to employ the complex form of the Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{\frac{i 2\pi n x}{\ell}} = \sum_{n=-\infty}^{+\infty} c_n e^{in\frac{\pi x}{a}}$$

We can also change from pure complex exponents to a normalized basis of $e^{\frac{in\pi x}{a}}/\sqrt{2a}$, $n = 0, \pm 1, \ldots$

That is

$$f(x) = \sum_{n=-\infty}^{+\infty} \underbrace{\left[\frac{1}{2a} \int_{-a}^{a} f(y)\, e^{-i\frac{\pi n y}{a}}\, dy \right]}_{c_n} e^{i\frac{n\pi x}{a}} =$$

$$= \sum_{n=-\infty}^{+\infty}{}' \left[\int_{-a}^{a} f(y)\, \frac{e^{-\frac{in\pi y}{a}}}{\sqrt{2a}}\, dy \right] \frac{e^{\frac{in\pi x}{a}}}{\sqrt{2a}}$$

If we define $\Delta k = \pi/a$, then after rearranging the last expression we obtain:

$$f(x) = \sum_{n=-\infty}^{+\infty}{}' \Delta k\, \frac{e^{in\Delta k x}}{\sqrt{2\pi}} \int_{-a}^{a} f(y)\, \frac{e^{-in\Delta k y}}{\sqrt{2\pi}}\, dy$$

By introducing the points $k_n = n\Delta k$, $n = 0, \pm 1, \pm 2, \ldots$ we partition the k axis into equally spaced subintervals of size $\Delta k = \frac{\pi}{a}$:

$$f(x) = \sum_{n=-\infty}^{+\infty} \Delta k\, \frac{e^{ik_n x}}{\sqrt{2\pi}} \underbrace{\int_{-a}^{a} \frac{e^{-ik_n y}}{\sqrt{2\pi}} f(y)\, dy}_{\tilde{f}(k_n)}$$

when $a \to \infty$ k_n essentially becomes a continuous variable, while $\Delta k \to dk$ (infinitely small interval), so that

$$f(x) = \int_{-\infty}^{+\infty} dk\, \frac{e^{ikx}}{\sqrt{2\pi}}\, \tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{f}(k)\, e^{ikx}\, dk \quad \leftarrow \text{inverse Fourier transform}$$

where $$\underbrace{\tilde{f}(k)}_{\text{Fourier image}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-ikx}\, dx \quad \leftarrow \text{Fourier transform}$$

Hence we can see that the Fourier transform is a limiting case of the Fourier series when $a \to \infty$.

Since the interval $[-a, a]$ approaches infinity we no longer need to make any assumptions about the periodicity like we did for the Fourier series.

It should be mentioned that there exist different conventions for the Fourier transform (and also for the Fourier series) in scientific literature. Physicists, mathematicians, and engineers tend to use different conventions for factors and signs in the exponents as well as for overall factors. In fact, in physics literature one can often encounter the following convention

$$\tilde{f}(k) = \int_{-\infty}^{+\infty} f(x)\, e^{-ikx}\, dx \qquad f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{f}(k)\, e^{ikx}\, dx$$

We will not use it!!! Instead we will stick to what we had above, where the $\frac{1}{2\pi}$ factor is split evenly between the direct and inverse Fourier transform:

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)\, e^{-ikx}\, dx \qquad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \tilde{f}(k)\, e^{ikx}\, dx$$

The advantages of this convention are that it is easier to remember and, more importantly, it preserves normalization of the Fourier image $\hat{f}(k)$. In other words, $\tilde{f}(k)$, which as we will learn later is the function in momentum representation, is automatically normalized. If $\int_{-\infty}^{+\infty} |f(x)|^2\, dx = 1$ then $\int_{-\infty}^{+\infty} |\tilde{f}(k)|^2\, dk = 1$.

The free particle

Let us now consider a particle moving in the potential that is zero everywhere, $V(x) \equiv 0$. The general solution of the corresponding Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad \text{or} \qquad \psi'' + k^2\psi = 0 \qquad k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

is

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

Here we do not have any boundary conditions. Adding the time dependence is trivial as $V \neq V(t)$ and it yields

$$\Psi(x,t) = A e^{ikx - \frac{iEt}{\hbar}} + B e^{-ikx - \frac{iEt}{\hbar}} = A e^{ik(x - \frac{\hbar k}{2m}t)} + B e^{-ik(x + \frac{\hbar k}{2m}t)}$$

The two terms represent two waves traveling in the positive and negative direction of the x-axis. The waves have a fixed profile (results from $x \pm vt$ dependence). In other words the shape of these waves does not change as they travel. We can account for the positive and negative travel direction by letting k run over negative and positive values, such that

$$\Psi(x,t) = A e^{i(kx - \frac{\hbar k^2}{2m}t)} = A e^{ik(x - \frac{\hbar k}{2m}t)}$$

The speed of the waves is

$$v_q = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$$

On the other hand the classical speed of a free particle with energy E is

$$v = \sqrt{\frac{2E}{m}} = 2v_q$$

Hence it appears that the quantum mechanical wave function travels twice slower.

Note also that the wave function is no longer normalizable:

$$\int_{-\infty}^{+\infty} \Psi_k^*(x,t)\, \Psi(x,t)\, dx = |A|^2 \int_{-\infty}^{+\infty} dx \rightarrow \infty$$

That means such states are not physically realizable. While it can be a useful mathematical idealization, there is no such a thing as a free particle with a definite energy E.

What can be done is that we can normalize our wave function (of a free particle) in such a way that there is a certain number of particles (say 1) in some volume V (volume in 1D). In many cases of practical calculations V will disappear due to cancellation.

The general solution to the time-dependent SE can be written as a linear combination

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)}\, dk$$

For an appropriate choice of $\phi(k)$ it can be normalized ($\frac{1}{\sqrt{2\pi}} \phi(k)\, dk$ plays the role of c_k in the discrete summation). However, any such choice would necessarily involve a range of k's (and hence a range of E's and velocities). Such a linear combination is called a wave pocket

The initial wave function is given by

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$

this is nothing but the inverse Fourier transform. Correspondingly

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ikx}\, dx$$

Now going back to the apparent paradox with v_q vs v_c (quantum velocity vs classical one), it turns out v_q represents a phase velocity (speed of individual ripples in a wave packet), while the speed of the envelope ($\phi(k)$) represents the group velocity. To determine the group velocity of

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk$$

regardless of the dispersion relation (in our case $\omega = \frac{\hbar k^2}{2m}$) we will assume that $\phi(k)$ is narrowly peaked about some value k_0 (almost free particle idealisation). In fact if it is not narrowly peaked then the whole idea of the group velocity v_g becomes vague. We Taylor expand $\omega(k)$ around k_0:

$$\omega(k) \approx \omega_0 + \omega_0'(k-k_0) + \ldots$$

Now we can write

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i((k_0+s)x - (\omega_0+\omega_0' s)t)}\, ds$$

where we used $s = k - k_0$

We can rewrite it as

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} e^{i(-\omega_0 t + k_0\omega_0' t)} \underbrace{\int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i((k_0+s)(x-\omega_0' t))}\, ds}_{\displaystyle \| \atop \displaystyle \Psi(x-\omega_0' t, 0)}$$

Hence,

$$\Psi(x,t) \approx e^{-i(\omega_0 - k_0\omega_0')t}\, \Psi(x-\omega_0' t, 0)$$

The phase factor, $e^{-i(\omega_0 - k_0\omega_0')t}$, won't change $|\Psi|^2$. It moves with the speed $v_g = \omega_0' = \frac{d\omega}{dk}$ (evaluated at $k=k_0$). This is different from the ordinary phase velocity $v_{phase} = \frac{\omega}{k}$

In our case $\omega = \frac{\hbar k^2}{2m}$

So

$$\frac{\omega}{k} = \frac{\hbar k}{2m}$$

at the same time $v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = 2 v_{phase}$.

This resolves the paradox.