Tutorial 3 - Fourier Transform and Wave Function

Mathematical Introduction

1. Inner product:
   Given two integrable functions $f(x)$ and $g(x)$ on the interval $[-L, L]$, the *inner product* is defined as follows,

$$\boxed{\langle g, f\rangle \equiv \int_{-L}^{L} g^*(x) f(x)\, dx}.$$

2. Discrete Fourier series:
   Given an integrable function $f(x)$ on the interval $[-L, L]$, one may expand it into an infinite series as follows,

$$\boxed{f(x) = \frac{1}{\sqrt{2L}} \sum_{n=-\infty}^{\infty} c_n e^{i\frac{\pi n x}{L}}}.$$

   Defining the *harmonic basis* or *modes* as

$$\varphi_n \equiv \frac{1}{\sqrt{2L}} e^{i\frac{\pi n x}{L}},$$

   it is easy to see that this basis is *orthogonal* with respect to inner product, that is

$$\langle \varphi_m, \varphi_n\rangle = \frac{1}{2L}\int_{-L}^{L} e^{i\frac{\pi n x}{L}} e^{-i\frac{\pi m x}{L}}\, dx = \delta_{nm}.$$

   It can be easily seen by looking at the integrand as

$$e^{i\frac{\pi n x}{L}} e^{-i\frac{\pi m x}{L}} = \left(\cos\left[(n-m)\frac{\pi x}{L}\right] + i\sin\left[(n-m)\frac{\pi x}{L}\right]\right),$$

   which leads to

$$n \neq m: \qquad \langle \varphi_m, \varphi_n\rangle \propto \cos\left[(n-m)\frac{\pi x}{L}\right] \text{ and } \sin\left[(n-m)\frac{\pi x}{L}\right]\Bigg|_{-L}^{L} = 0,$$

$$n = m: \qquad \langle \varphi_m, \varphi_n\rangle = 1.$$

   Using orthonormality of the basis functions we may calculate the *harmonic coefficients* as follows,

$$\begin{aligned}
\frac{1}{\sqrt{2L}}\int_{-L}^{L} f(x) e^{-i\frac{\pi n x}{L}}\, dx &= \frac{1}{2L}\int_{-L}^{L} \sum_{m=-\infty}^{\infty} c_n e^{i\frac{\pi m x}{L}} e^{-i\frac{\pi n x}{L}}\, dx \\
&= \sum_{m=-\infty}^{\infty} c_m \frac{1}{2L}\int_{-L}^{L} e^{i\frac{\pi m x}{L}} e^{-i\frac{\pi n x}{L}}\, dx \\
&= \sum_{m=-\infty}^{\infty} c_m \delta_{nm}
\end{aligned}$$

   thus,

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

In addition, one can use the decomposition of the exponent and write

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left[a_n \cos \frac{\pi n x}{L} + b_n \sin \frac{\pi n x}{L} \right],$$

where

$$\begin{aligned} a_0 &= \frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x)\, dx, \\ a_n &= \frac{1}{\sqrt{L}} \int_{-L}^{L} f(x) \cos \frac{\pi n x}{L} dx, \\ b_n &= \frac{1}{\sqrt{L}} \int_{-L}^{L} f(x) \sin \frac{\pi n x}{L} dx. \end{aligned}$$

3. Fourier transform:
   Given an integrable function $f(x)$ defined on all space, it is not possible to represent it as a discrete sum of harmonics, but rather as a continuous harmonic basis. In order to do that we take the continuous limit, by defining the mode *wavenumber* $k \equiv \pi n / L$ such that $\Delta k = \pi \Delta n / L$

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2L}} \sum_n c_n e^{i \frac{\pi n x}{L}} \left(\frac{\Delta n}{1} \right) = \frac{1}{\sqrt{2L}} \sum_k \frac{L}{\pi} \left[\frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x') e^{-ikx'} dx' \right] e^{ikx} \Delta k \\ &= \frac{1}{\sqrt{2\pi}} \sum_k \underbrace{\left[\frac{1}{\sqrt{2\pi}} \int_{-L}^{L} f(x') e^{-ikx'} dx' \right]}_{g(k)} e^{ikx} \Delta k, \end{aligned}$$

   and taking the limit of $L \to \infty$, $\Delta k \to dk$ and $\sum \to \int$, we find

$$\boxed{\begin{aligned} f(x) &= \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \\ g(k) &= \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \end{aligned}},$$

   where $g(k) = \mathcal{F}[f(x)]$ is called the *Fourier transform* of $f(x)$.

4. Dirac's delta function:
   Writing the Fourier transform explicitly

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx} dk \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left(\int_{-\infty}^{\infty} f(y) e^{-iky} dy \right) e^{ikx} dk \\ &= \int_{-\infty}^{\infty} f(y)\, dy \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} dk, \end{aligned}$$

   we can define the Dirac delta function as

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

   such that

$$\boxed{\int_{-\infty}^{\infty} f(y)\, \delta(x-y)\, dy = f(x)}.$$

   It is easy to show that

$$\delta(ax) = \frac{1}{|a|} \delta(x) \quad \text{and} \quad \delta(-x) = \delta(x).$$

5. Polynomial expansion:
In a similar manner to harmonic functions, one may expand a function $f(x)$, defined on Ω, in terms of an orthonormal polynomial basis $P_n(x)$, which satisfies

$$\langle P_m(x), P_n(x)\rangle = \int_\Omega P_m^*(x) P_n(x) \omega(x) dx = \delta_{mn},$$

where $\omega(x)$ is a weight function that is introduced in order to normalize the basis (in harmonic functions $\omega(x) = 1$). Therefore

$$\boxed{f(x) = \sum_n a_n P_n(x), \quad x \in \Omega},$$

where

$$\boxed{a_n = \langle P_n(x), f(x)\rangle = \int_\Omega P_n^*(x) f(x) \omega(x) dx}.$$

The Dirac delta function is easily found from

$$\begin{aligned} f(x) &= \sum_n a_n P_n(x) \\ &= \int_\Omega f(y) dy \sum_n P_n(x) P_n^*(y) \omega(y) \end{aligned}$$

$$\boxed{\delta(x-y) = \sum_n P_n(x) P_n^*(y) \omega(y)}.$$

Some relevant polynomials:

Name	Sym.	$\omega(x)$	Ω
Lagendre	$\mathcal{L}_n(x)$	1	$[-1, 1]$
Hermite	$H_n(x)$	e^{-x^2}	$[-\infty, \infty]$
Laguerre	$L_n^l(x)$	$x^k e^{-x}$	$[0, \infty]$

Question 1:

Find the Fourier coefficients for the function $f(x) = x$ on the interval $[-\pi, \pi]$.

Solution:

Using the expansion to in Fourier modes

$$\varphi_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx},$$

we find

$$c_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} x e^{-inx} dx.$$

Note that for $n = 0$ the integral is

$$c_0 = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} x dx = 0,$$

whereas for $n \neq 0$ we will use a useful trick for solving the integral by defining $\alpha = in$,

$$\begin{aligned} \int_{-\pi}^{\pi} x e^{-\alpha x} dx &= -\frac{d}{d\alpha} \int_{-\pi}^{\pi} e^{-\alpha x} dx \\ &= \frac{d}{d\alpha} \left[\frac{1}{\alpha}\left(e^{-\alpha\pi} - e^{\alpha\pi}\right)\right] \\ &= -\frac{1}{\alpha^2} \underbrace{\left(e^{-\alpha\pi} - e^{\alpha\pi}\right)}_{-2i \sin n\pi} + \frac{\pi}{\alpha} \underbrace{\left(-e^{-\alpha\pi} - e^{\alpha\pi}\right)}_{-2\cos n\pi}, \end{aligned}$$

then

$$c_n = \frac{1}{\sqrt{2\pi}}\frac{i}{n}\left[\underbrace{\cos n\pi}_{(-1)^n} - \underbrace{\frac{\sin n\pi}{n\pi}}_{0}\right] = \frac{1}{\sqrt{2\pi}}\frac{i}{n}(-1)^n \quad \forall n \neq 0.$$

Therefore

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}}\sum_{n\neq 0}\frac{i}{n}(-1)^n e^{inx} \\ &= \frac{1}{\sqrt{2\pi}}\sum_{n=1}^{\infty}\frac{i}{n}(-1)^n\left(e^{inx} - e^{-inx}\right), \end{aligned}$$

$$\boxed{f(x) = \sum_{n=1}^{\infty}\frac{\sqrt{2}}{n\sqrt{\pi}}(-1)^{n+1}\sin nx}.$$

Question 2:

Find the Fourier transform of the function

$$\varphi(x) = \begin{cases} c, & -a < x < a \\ 0 & \text{else} \end{cases}.$$

Solution:

Taking the Fourier transform of $\varphi(x)$ yields

$$\begin{aligned} \tilde{\varphi}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\varphi(x)\,e^{-ikx}dx \\ &= \frac{1}{\sqrt{2\pi}}\int_{-a}^{a} ce^{-ikx}dx \\ &= \frac{c}{\sqrt{2\pi}ik}\left(e^{ika} - e^{-ika}\right) \end{aligned}$$

$$\boxed{\tilde{\varphi}(k) = c\sqrt{\frac{2}{\pi}}\frac{\sin ka}{k}}.$$

Question 3:

Find the Fourier transform of the Gaussian function

$$g(x) = \frac{1}{\sigma}e^{-\frac{x^2}{2\sigma^2}}.$$

Solution:

Taking the Fourier transform of $g(x)$ yields

$$\begin{aligned} \tilde{g}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x)\,e^{-ikx}dx \\ &= \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}e^{-ikx}dx. \end{aligned}$$

Looking at the power of the exponent we can write

$$-\frac{1}{2\sigma^2}\left(x^2 + 2i\sigma^2 kx\right) = -\frac{1}{2\sigma^2}\left(x^2 + 2i\sigma^2 kx - \sigma^4 k^2\right) - \frac{\sigma^2 k^2}{2},$$

which leads to

$$\tilde{g}(k) = \frac{e^{-\sigma^2 k^2/2}}{\sqrt{2\pi}\sigma}\underbrace{\int_{-\infty}^{\infty} e^{-\frac{u^2}{2\sigma^2}}du}_{I},$$

where we defined $u = x + i\sigma^2 k$. we are left with a simple Gaussian integral I which can be solved as follows

$$I^2 = \left(\int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx\right)^2 = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma^2}} dy = \int_{-\infty}^{\infty} e^{-\frac{x^2+y^2}{2\sigma^2}} dxdy$$

moving to polar coordinates

$$I^2 = \int_0^{2\pi} \int_0^{\infty} e^{-\frac{r^2}{2\sigma^2}} r dr d\varphi = \pi \int_0^{\infty} e^{-\frac{\xi}{2\sigma^2}} d\xi = 2\pi\sigma^2,$$

where we defined $\xi = r^2$ hence $d\xi = 2rdr$, which gives $I = \sqrt{2\pi\sigma^2}$.
Therefore

$$\boxed{\tilde{g}\left(k\right) = e^{-\frac{\sigma^2 k^2}{2}}}.$$

This is a Gaussian with width of $\tilde{\sigma} = 1/\sigma$.

Wave function

A wave function is a mathematical description of the state of a system, through which one may infer probabilistic features of measurable quantities of the system.
Features of wave function:

- Superposition: If ψ_1 and ψ_2 are wave functions then $\psi = \psi_1 + \psi_2$ is a wave function as well.
- Probabilistic interpretation: The probability density of measuring the position of a particle around a point x at time t is given by

$$\rho\left(\boldsymbol{x}, t\right) = \psi^*\left(\boldsymbol{x}, t\right)\psi\left(\boldsymbol{x}, t\right) = \left|\psi\right|^2, \quad \text{s.t.} \quad \int_\Omega \rho\left(\boldsymbol{x}, t\right) d\boldsymbol{x} = 1.$$

- Spectral decomposition: Every wave function can be described by the sum of states that form a basis in Hilbert space (e.g. Fourier series).

Time evolution of the wave function

Given the initial wave function $\psi\left(\boldsymbol{x}, 0\right)$, how does one evolve it to $\psi\left(\boldsymbol{x}, t\right)$? Consider the representation of a plane wave, which propagates to the positive or negative x direction, by

$$\varphi\left(x, t\right) \propto \cos\left(kx - \omega t + \alpha\right) \qquad \text{or} \qquad \varphi\left(x, t\right) \propto \cos\left(kx + \omega t + \beta\right),$$

it is clear that, for some given initial conditions at $\varphi\left(x, 0\right)$ for which $\alpha = \beta = 0$, the two are identical, thus we are unable to differentiate between waves that propagate left and right. A simple example is vibrations of a string, for which we typically require to know $\dot{\varphi}\left(x, t = 0\right)$ as well, as the differential equation that describe the system is of second order. This concludes that we must choose between

1. $\varphi\left(\boldsymbol{x}, 0\right)$ alone does not determine $\varphi\left(\boldsymbol{x}, t\right)$.
2. $\varphi\left(\boldsymbol{x}, 0\right)$ alone does determine $\varphi\left(\boldsymbol{x}, t\right)$, but the description of a simple harmonic plane wave is different than above.

Since in quantum physics we cannot observe the waves directly, we limit ourselves to the second option, then we must find some other description for a plane wave by taking the general case of

$$\varphi_1\left(x, t\right) \propto \cos\left(kx - \omega t\right) + \delta_1 \sin\left(kx - \omega t\right) \qquad \text{and} \qquad \varphi_2\left(x, t\right) \propto \cos\left(kx + \omega t\right) + \delta_2 \sin\left(kx + \omega t\right),$$

for plane waves that propagate in different directions. Requiring that φ_1 and φ_2 are linearly independent will ensure that any plane wave can be expressed as the combination of the two. Therefore, a free particle moving in the positive x direction must be always described by φ_1 only, at time t as well as at $t = 0$, hence

$$\cos\left(kx + \varepsilon\right) + \delta_1 \sin\left(kx + \varepsilon\right) = a_1\left(\varepsilon\right)\left(\cos kx + \delta_1 \sin kx\right) \quad \forall\, x \text{ and } \varepsilon.$$

Using the identities, $\cos\left(u \pm v\right) = \cos u \cos v \mp \sin u \sin v$ and $\sin\left(u \pm v\right) = \sin u \cos v \pm \cos u \sin v$, this equation leads to

$$\cos kx \cos\varepsilon - \sin kx \sin\varepsilon + \delta_1\left[\sin kx \cos\varepsilon + \cos kx \sin\varepsilon\right] = a_1\left(\varepsilon\right)\left(\cos kx + \delta_1 \sin kx\right),$$

$$\cos\varepsilon + \delta_1 \sin\varepsilon = a_1(\varepsilon) \quad \text{and} \quad \delta_1 \cos\varepsilon - \sin\varepsilon = a_1(\varepsilon)\,\delta_1 \quad \forall\,\varepsilon,$$

which can be solved for δ_1 as

$$\cos\varepsilon + \delta_1^2(\cos\varepsilon - a_1) = a_1 \quad \rightarrow \quad \delta_1^2 = -1 \quad \text{or} \quad \delta_1 = \pm i.$$

Similarly for a free particle propagating in the negative x direction we find $\delta_2 = \pm i$. Choosing $\delta_1 = i$ and $\delta_2 = -i$ as convention, we come to the conclusion that in order for $\varphi(\boldsymbol{x}, t)$ to be determined solely by $\varphi(\boldsymbol{x}, 0)$ we must extend the wave φ to be a complex valued function such that

$$\varphi_1(x,t) = Ae^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} \quad \text{and} \quad \varphi_2(x,t) = Be^{-i(\boldsymbol{k}\cdot\boldsymbol{x}+\omega t)}$$

Therefore, the description of the time evolution of the wave function is

$$\psi(\boldsymbol{x},t) = \int_{\tilde{\Omega}} \tilde{\psi}(\boldsymbol{k})\, e^{i(\boldsymbol{k}\cdot\boldsymbol{x}-\omega t)} d\boldsymbol{k},$$

where each plane wave evolve in time with different frequency $\omega(k)$ (a.k.a. dispersion relation), which is determined by the equations of motion.

Question 4:

Given the initial Gaussian wave function

$$\psi(x,0) = Ae^{-\frac{x^2}{2a^2}},$$

and the dispersion relation $\omega(k) = \hbar k^2/2m$. Find

1. The normalization $|A|$.
2. The Fourier transform $\tilde{\psi}(k)$.
3. The time dependent wave function $\psi(x,t)$.

Solution:

1. Using the probability normalization condition at $t = 0$

$$\int_{\Omega} \rho(x,0)\, dx = 1,$$

we find

$$\int_{\Omega} \psi^*(x,0)\,\psi(x,0)\, dx = |A|^2 \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2}} dx = |A|^2 \sqrt{\pi a^2}.$$

Therefore

$$\boxed{|A| = \left(\frac{1}{a\sqrt{\pi}}\right)^{1/2}}.$$

2. Taking the Fourier transform of $\psi(x,0)$ yields

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{\Omega} \psi(x,0)\, e^{-ikx} dx = \frac{A}{2\pi} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2a^2}} e^{-ikx} dx,$$

using the results for Fourier transform of a Gaussian from previous exercise,

$$\boxed{\tilde{\psi}(k) = \sqrt{a}\pi^{7/4} e^{-\frac{k^2a^2}{2}}}.$$

3. The time dependent wave function is simply

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\tilde{\Omega}} \tilde{\psi}(k)\, e^{i(kx-\omega t)} dk = \int_{-\infty}^{\infty} \frac{\sqrt{a}}{\sqrt{2}} \pi^{5/4} e^{-\frac{k^2a^2}{2}} e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)} dk.$$

In order to solve the integral let us define $\tau \equiv \hbar t/2m$, so we get

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{\infty} \frac{\sqrt{a}}{\sqrt{2}} \pi^{5/4} e^{-\left(\frac{a^2}{2}+i\tau\right)k^2+ikx} dk \\
&= \frac{\sqrt{a}}{\sqrt{2}} \pi^{5/4} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(a^2+2i\tau\right)\left(k^2-2\frac{ikx}{a^2+2i\tau}\right)} dk \\
&= \frac{\sqrt{a}}{\sqrt{2}} \pi^{5/4} e^{-\frac{1}{2}\frac{x^2}{a^2+2i\tau}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\left(a^2+2i\tau\right)\left(k-\frac{ix}{a^2+2i\tau}\right)^2} dk \\
&= \frac{\sqrt{a}}{\sqrt{2}} \pi^{5/4} e^{-\frac{1}{2}\frac{a^2-2i\tau}{a^4+4\tau^2}x^2} \sqrt{\frac{2\pi}{\left(a^2+2i\tau\right)}}
\end{aligned}$$

$$\boxed{\psi(x,t) = \frac{\pi^{7/4}\sqrt{a}}{\sqrt{a^2+i\hbar t/m}} e^{-\frac{1}{2}\frac{a^2-i\hbar t/m}{a^4+\hbar^2 t^2/m^2}x^2}}.$$

Another way to get this result is by defining the Fourier transform of a *propagator* $\tilde{P}(k,t) \equiv e^{-i\omega(k)t}$ so that

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\tilde{\Omega}} \tilde{\psi}(k)\, \tilde{P}(k,t)\, e^{ikx} dk,$$

that is, the time dependent wave function is the convolution between the initial wave function and a propagator

$$\psi(x,t) = \psi(x,0) * P(x,t),$$

where

$$P(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\tilde{\Omega}} \tilde{P}(k,t)\, e^{ikx} dk,$$

Therefore

$$\psi(x,t) = \psi(x,0) * P(x,t) = \int \psi(y,0)\, P(x-y,t)\, dy.$$

In our case

$$P(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\tilde{\Omega}} \tilde{P}(k,t)\, e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega t} e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\frac{\hbar k^2}{2m}t} e^{ikx} dk,$$

again, using the gaussian Fourier transform

$$P(x,t) = \sqrt{\frac{m}{i\hbar t}} e^{i\frac{x^2}{2\hbar t/m}}.$$

Question 5:

Consider the double slits experiment with electrons, in which the electrons that pass through the first slit gain a random phase ϕ. What would be the interference pattern?

Solution:

The wave functions superposition is $\psi = e^{i\phi}\psi_1 + \psi_2$, which leads to amplitude

$$|\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + e^{-i\phi}\psi_1^*\psi_2 + e^{i\phi}\psi_1\psi_2^*.$$

Using the decomposition to real and imaginary, $\psi_1^*\psi_2 = \mathrm{Re}\left[\psi_1^*\psi_2\right] + \mathrm{Im}\left[\psi_1^*\psi_2\right]$, yields

$$\begin{aligned}
|\psi|^2 &= |\psi_1|^2 + |\psi_2|^2 + e^{-i\phi}\left(\mathrm{Re}\left[\psi_1^*\psi_2\right] + i\mathrm{Im}\left[\psi_1^*\psi_2\right]\right) + e^{i\phi}\left(\mathrm{Re}\left[\psi_1^*\psi_2\right] - i\mathrm{Im}\left[\psi_1^*\psi_2\right]\right) \\
&= |\psi_1|^2 + |\psi_2|^2 + 2\mathrm{Re}\left[\psi_1^*\psi_2\right]\cos\phi + 2\mathrm{Im}\left[\psi_1^*\psi_2\right]\sin\phi.
\end{aligned}$$

Averaging over the random phase we see that the cross terms vanish leaving only

$$I \sim \frac{1}{2\pi} \int_0^{2\pi} |\psi|^2 d\phi = |\psi_1|^2 + |\psi_2|^2,$$

which means there is no interference!