Tutorial 2 - Wave Function

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

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

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

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

it is clear that, for some given initial conditions at $\varphi(x, 0)$ 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 $\dot{\varphi}(x, t = 0)$ as well, as the differential equation that describe the system is of second order. This concludes that we must choose between

1. $\varphi(\boldsymbol{x}, 0)$ alone does not determine $\varphi(\boldsymbol{x}, t)$.
2. $\varphi(\boldsymbol{x}, 0)$ alone does determine $\varphi(\boldsymbol{x}, t)$, 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

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

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

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

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

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

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

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 1:

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

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

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

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

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

The double slits experiment

Consider a projection of coherent monochromatic light onto a plate with 2 slits separated by distance d. A distance L from the plate is located a screen.

- If light is a particle we'd expect two slits image on the screen, corresponding to the deterministic trajectory of the light particles (photons).
- If light is a wave we'd expect an interference pattern on the screen.

The results of the experiment coincide with the second proposition, does that mean that light is a wave? Slowing down the photons rate (by reducing the light intensity) we are able to observe the discrete spots on the screen, i.e. light travels in discrete packets - is it a particle?
Waiting long enough we find that the discrete spots form a interference pattern! The logical conclusion is that light is a particle that interferes with itself, neither a wave nor a particle.
The same results are reproduced with electrons instead of photons, and conceptually all other particles share this feature.

Question 2:

Consider the double slits experiment with photons, only this time the wavelength of the photons is gradually increased. What would be the wavelength for which there wont be visible interference?

Solution:

The wave functions that correspond to photons from each slit are

$$\psi_1(r_1) = Ae^{i(kr_1-\omega t)} \quad \text{and} \quad \psi_2(r_2) = Ae^{i(kr_2-\omega t)}.$$

Considering the wave function at a point on the screen, we have the superposition of light from both slits, that is

$$\psi = \psi_1 + \psi_2,$$

so that the observed intensity on the screen is simply

$$I \sim |\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + \psi_1^*\psi_2 + \psi_1\psi_2^* \propto 2 + e^{-ik(r_1-r_2)} + e^{ik(r_1-r_2)} = 2\left(1+\cos\left[k\left(r_1-r_2\right)\right]\right) \sim \cos^2\left[\frac{k}{2}\left(r_1-r_2\right)\right],$$

which can be written in terms of $r_1 - r_2 = d\sin\theta$,

$$I \sim \cos^2\left(\frac{kd\sin\theta}{2}\right),$$

which vanishes when

$$\frac{kd\sin\theta}{2} = (2n+1)\frac{\pi}{2}, \quad n = 0, \pm1, \pm2\ldots$$

This equation describes the destructive interference lines, for which the 0th order is

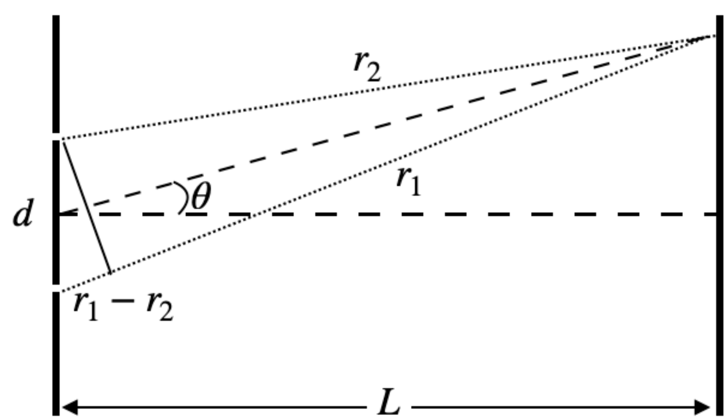
$$kd\sin\theta = \pi.$$

In order for the 0th order to be outside the screen (i.e. all the other interference orders will be out as well) we require $\theta_c = \pi/2$, which leads to

$$\sin\theta = \frac{\lambda}{2d}$$

$$k_c = \frac{2\pi}{\lambda} = \frac{\pi}{d} \quad \rightarrow \quad \lambda_c = 2d,$$

thus, if $\lambda < 2d$ we will see the interference patter, while for $\lambda \geq 2d$ we will not see it.



Question 3:

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!