
Lecture 3

The Wavefunction

Assigned Reading:

E&R	1 _{6,7} , 2 _{1,2,3,4,5} , 3 _{all} NOT 4 _{all} !!!
Li.	1 _{all} , 2 _{3,5,6} NOT 2-4!!!
Ga.	1 _{2,3,4} NOT 1-5!!!
Sh.	3

In classical mechanics, the configuration or *state* of a system is given by a point (\mathbf{x}, \mathbf{p}) in the space of coordinates and momenta. This specifies everything else in the system in a fully deterministic way, in that any observable Y that can be expressed as $Y(\mathbf{x}, \mathbf{p})$ can be found, and any that cannot is irrelevant. Yet, as we have seen with the diffraction of electrons, it is impossible to know both the position and momentum of the electron exactly at every point along the trajectory. This is mathematically expressed as the famous *position-momentum uncertainty principle*:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (0.1)$$

Hence, specifying a state by (\mathbf{x}, \mathbf{p}) clearly will not work. So what specifies the state of a quantum system?

The configuration or *state* of a quantum object is completely specified by a *wavefunction* denoted as $\psi(x)$.

And what does $\psi(x)$ mean?

$p(x) = |\psi(x)|^2$ determines the probability (density) that an object in the state $\psi(x)$ will be found at position x .

Note that

$$\psi \in \mathbb{C},$$

meaning the wavefunction is complex! Here, the real part of ψ is being drawn for simplicity, as complex-plane paper is hard to find. Furthermore, ψ must be singly-valued and not “stupid”; the latter point will be elaborated later.

Let us examine this set of examples in further detail. The first wavefunction ψ_1 is sharply peaked at a particular value of x , and the probability density, being its square, is likewise peaked there as well. This is the wavefunction for a particle well localized at a position given by the center of the peak, as the probability density is high there, and the width of the peak is small, so the uncertainty in the position is very small.

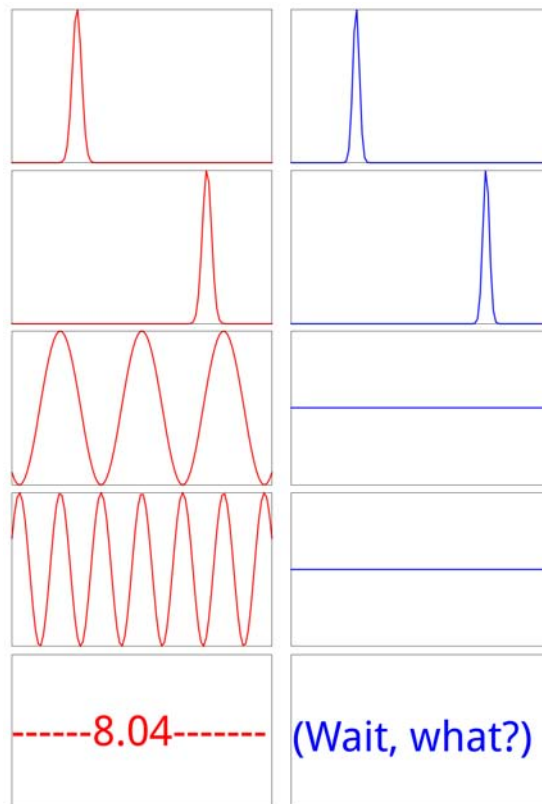


Figure 1: Examples of wavefunctions (red, left) and corresponding probability densities (blue, right)

The second wavefunction ψ_2 has the same peak profile, but shifted to a different position center. All of the properties of the first wavefunction hold here too, so this simply describes a particle that is well-localized at that different position.

The third and fourth wavefunctions ψ_3 and ψ_4 respectively look like sinusoids of different spatial periods. The wavefunctions are actually complex of the form

$$\psi(x) = Ne^{ikx},$$

so only the real part is being plotted here. Note that even though the periods are different,

$$|e^{ikx}|^2 = 1$$

for all k , so the corresponding probability densities are the same except for maybe a normalization constant. We saw before that it does not make a whole lot of sense to think of a sinusoidal wave as being localized in some place. Indeed, the positions for these two wavefunctions are ill-defined, so they are not well-localized, and the uncertainty in the position is large in each case.

The fifth wavefunction is multiply-valued, so it is considered to be “stupid”. It does not have a well-defined probability density.

Note the normalization and dimensions of the wavefunction: the cumulative probability over all possible positions is unity, so

$$\int |\psi(x)|^2 dx = 1,$$

and the probability density has dimensions reciprocal to the integration variable that yields a cumulative probability which in this case is position, so the wavefunction has units of reciprocal square root of length. Finally, note that while the wavefunction is in general complex, the probability (density) must always be real. This also means that $\psi(x)$ is only uniquely defined up to an arbitrary complex phase, because all imaginary exponentials $e^{i\theta}$ satisfy $|e^{i\theta}|^2 = 1$, so the probability density and therefore the physical interpretation of the wavefunction are unaffected by multiplication by a complex phase.

You may now be thinking that the only useful wavefunctions are peaks that are well-localized around a given position. But let us remember that the de Broglie relations says that a wave of wavelength λ has a momentum $p = h\lambda^{-1}$. This means that ψ_3 and ψ_4 , being sinusoidal waves, have well-defined wavelengths and therefore well-defined momenta with small uncertainties in their respective momenta, with ψ_4 having a smaller wavelength and therefore a larger momentum than ψ_3 . On the other hand, ψ_1 and ψ_2 do not look like sinusoidal waves, so it is difficult to define a wavelength and therefore a momentum for each, and the respective momentum uncertainties are large. These qualitatively satisfy the uncertainty relation.

In general, given a wavefunction, once the uncertainty in the position is determined, a lower bound for the uncertainty in the momentum can be found by the uncertainty relation. This always works. If Δx is large, then Δp is small, and the opposite is true as well. At some point, we will have to figure out how to calculate these uncertainties. But there are two things to be done before that.

The first is a point of notation. A plane wave

$$\psi(x, t) = e^{i(kx - \omega t)}$$

has frequency

$$\omega = 2\pi\nu$$

and wavevector

$$k = 2\pi\lambda^{-1}.$$

This means that the de Broglie relations can be rewritten as

$$E = \hbar\omega \tag{0.2}$$

$$p = \hbar k. \tag{0.3}$$

In three dimensions, the energy relation is unchanged, while the momentum relation $\mathbf{p} = \hbar\mathbf{k}$ simply takes on the form of a vector relation.

The second is much more important, and that is to quantify the notion of superposition that we have been developing.

Given two possible states of a quantum system corresponding to two wavefunctions ψ_a and ψ_b , the system could also be in a superposition $\psi = \alpha\psi_a + \beta\psi_b$ with α and β as arbitrary complex coefficients satisfying normalization.

This forms the soul of quantum mechanics!

Note that for a superposition state

$$\psi(x) = \alpha\psi_a(x) + \beta\psi_b(x),$$

the probability density

$$\mathbf{p}(x) = |\alpha\psi_a(x) + \beta\psi_b(x)|^2 = |\alpha\psi_a(x)|^2 + |\beta\psi_b(x)|^2 + \alpha^*\beta\psi_a^*(x)\psi_b(x) + \alpha\beta^*\psi_a(x)\psi_b^*(x)$$

exhibits quantum interference aside from the usual addition of probability!

For example, let us consider $\psi_5 = \psi_1 + \psi_2$ from our previous set of examples. Putting normalization aside, this looks like two distinct well-localized peaks. Each peak individually represented a particle that was localized at the position of the peak center. But now that there are two peaks, the particle is at neither position individual. It is not at both positions simultaneously, nor is it at no position at all. It is simply in a superposition of two states of definite position. The probability density of this superposition state will show no interference because when one of the component wavefunctions exhibits a peak, the other component wavefunction is zero, so their product is zero at all positions.

Similarly, $\psi_6 = \psi_3 + \psi_4$ is a superposition of two states of definite momentum. It cannot be said that a particle in this state has one or the other momentum, nor can it be said that it has both or neither momenta. In contrast to the previous superposition example, though, the probability density will exhibit interference because the product of the two wavefunctions is not always zero as they are both sinusoidal waves.

Note for the example of ψ_5 that this superposition state has more spatial localization than each of the component sinusoidal wavefunctions. This spatial localization could be made even better with three states of different definite momenta. We could do this for arbitrarily large countable n : as a state of definite momentum is

$$\psi(x; k) = e^{ikx}$$

except for normalization, a superposition of states of definite momentum

$$\psi = \sum_j \alpha_j e^{ik_j x}$$

could have a very well-localized position center. Or, other states with different properties compared to just having a well-localized position could be built from superpositions of momentum states. But why should we stop there? There is no reason to consider only discrete k_j , when the entire range of k over the real line is available.

The Fourier theorem says that any function $f(x)$ can be composed of complex sinusoidal waves e^{ikx} as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk. \quad (0.4)$$

This is the continuous analogue of the discrete sum Fourier series

$$f(x) = \sum_j \alpha_j e^{ik_j x}. \quad (0.5)$$

Furthermore, given $f(x)$, we can compute the Fourier transform

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx. \quad (0.6)$$

This is the continuous analogue of the Fourier expansion coefficients

$$\alpha_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ik_j x} dx. \quad (0.7)$$

The physical interpretation of this is that any wavefunction $\psi(x)$ can be expressed as a *superposition* of states e^{ikx} with definite momenta $p = \hbar k$ as

$$\boxed{\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}(k) e^{ikx} dk.} \quad (0.8)$$

Furthermore, $\tilde{\psi}(k)$ gives the exact same information as $\psi(x)$ about the quantum state, so once one is known, the other can be found automatically as well.

What do the Fourier transforms of wavefunctions look like? Let us look at the previous set of examples. ψ_1 looks like a Dirac delta function, and its Fourier transform is a complex exponential ... except that is exactly what ψ_3 looks like as a function of x ! Similarly, ψ_2 has a larger position than ψ_1 , so its Fourier transform has a larger frequency as a complex exponential function of k . Furthermore, performing the Fourier transform on a function

twice simply recovers the original function. This implies that the Fourier transform of ψ_3 looks like ψ_1 as a function of k , and the same goes for ψ_4 with regard to ψ_2 . Finally, in a similar vein, aside from normalization, ψ_5 and ψ_6 are Fourier transforms of each other.

This means that a wavefunction that is well-localized around a given position has a Fourier transform that looks like a sinusoidal function of k , and the frequency of oscillation as a function of k is given by that position. Similarly, a wavefunction that looks like a sinusoidal function of x has a Fourier transform that is well-localized around a given wavevector, and that wavevector is the frequency of oscillation as a function of x .

So what then is $\mathbf{p}(k)$? This is the probability density that the particle described by the wavefunction $\psi(x)$ has a momentum $p = \hbar k$. The expression turns out to be surprisingly simple:

$$\mathbf{p}(k) = |\tilde{\psi}(k)|^2,$$

and it is not too difficult to show this to be the case.

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