1 Probability amplitude versus Probability density versus just Probability

Wavefunction components are not probabilities themselves; they are **probability amplitudes**. This means, you have to take their absolute square (modulus square) in order to get something like a probability.

If you take the absolute square, do you get a **probability**, or a **probability density**? This depends on how the underlying Hilbert space is indexed. If it is a discrete index, you get a probability. If it is a continuous index, you get a probability density.

There are thus three types of quantities — amplitudes of probability, probability densities, and discrete probabilities — to get used to. You may have met probability densities and discrete probabilities in statistics class; I review these below as well. The concept of probability amplitudes is specific to quantum mechanics.

2 Probability density vs Probability

We first remind ourselves of the difference between a probability and a probability density, as you might have learned them in a statistics module. This section is not really about quantum mechanics, yet.

Imagine a statistical variable (random variable), that can take a discrete number of values. For example, a throw of a die can result in one of six results. An index running over these values will be a **discrete** index. Each of the results ('events') is associated with a probability. For example, we could write the individual probabilities, in obvious notation, as

$$P_1 = 0.2 \quad P_2 = 0.1 \quad P_3 = 0.1 \quad P_4 = 0.25 \quad P_5 = 0.2 \quad P_6 = 0.15 \, .$$

(Clearly this is not a fair die, as the probabilities are unequal. Biased!)

This listing provides the (discrete) probability distribution. P_i is the probability of obtaining the outcome i. The probabilities must satisfy

$$\sum_i P_i = 1 \, .$$

Now consider a **continuous** random variable, e.g., the height of a randomly selected person in the Dublin area, or the y-component of the position of an object. The value of the height or position is a continuous variable, i.e., we could not possibly hope to list all possible values. So we can't hope to write a discrete list of probabilities as we did in the discrete case. Instead, the probability distribution can only be specified as a function

$$P(y)$$

that has a continuous argument, or a continuous index. The variable y could be the height or position in the above examples. It takes a continuum of values, an infinite number of rational and irrational values, which you cannot list exhaustively.

So how do you interpret this function $P(y)$? It would be imprecise to say that $P(y_0)$ it is the probability of the height being **exactly** $y = y_0$. The probability of finding exactly a particular value is actually zero. The proper interpretation is to consider the function $P(y)$ to be a **probability density**. You can use this function to obtain probabilities of finding a value within an interval. For example, if $P(y)$ is the **probability density**, then the **probability** of obtaining a value in the interval $y \in [a, b]$ is

$$\int_a^b P(y)dy.$$

Informally, you could say that $P(y)dy$ gives you the probability of finding a value in the interval $(y, y + dy)$. You probably shouldn't say that in math class, but it's perfectly appropriate for physics discussions.

Note: In our discrete example (die) there were only six possible values of the index. However, the underlying index could be discrete but yet have an **infinite** number of possible values.
For example, you could ask what is the probability of finding n stars in a randomly chosen galaxy. You could try listing the probabilities P_n

$$P_0,\ P_1,\ P_2,\ P_3,\ \ldots$$

The list is discrete but infinite. It never ends because galaxies could in principle be arbitrarily large. The index n is discrete, nevertheless it has an infinite number of possible values. Because n is discrete, you use discrete **probabilities** (and not a **probability density** function) to describe the probability distribution.

You also know such examples from quantum mechanics: imagine listing the probabilities of finding a particle in a harmonic oscillator in the state $n = 0$, $n = 1$, $n = 2$,.... The list is discrete; you have probabilities instead of a probability density. However the list in infinite.

3 Probabilities vs Probability densities in quantum mechanics

In quantum mechanics, the underlying Hilbert space might be finite-dimensional or infinite-dimensional. If it is finite-dimensional, states will be indexed by a finite and therefore discrete set. If the Hilbert space in infinite-dimensional, states might be indexed by either continuous variables or by discrete indices! Let us give examples of each below.

3.1 Finite Hilbert space – discrete indexing

The example we have looked at repeatedly is a two-state system, namely a spin-$\frac{1}{2}$ system. Let us express wavefunctions in the usual basis $\{|\uparrow\rangle, |\downarrow\rangle\}$. Then the wavefunction is a two-component vector:

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \qquad \text{with} \quad \sum_i |c_i|^2 = 1.$$

The index i is discrete, not continuous. So there are no probability densities appearing in this system, only probabilities.

In particular, $|c_1|^2$ is the probability of finding the z-component of the spin to be positive $(+1/2)$, and $|c_2|^2$ is the probability of finding the z-component of the spin to be negative $(-1/2)$. The sum of these probabilities is 1, because these are the only possible values that can appear in a measurement of S_z.

Here is a second example. Imagine an electron on a molecule. The structure of the molecule is such that there are only 4 orbitals (states) available for the electron. Let us call these states $|A\rangle$, $|B\rangle$, $|C\rangle$, $|D\rangle$. ($|A\rangle$ is the state of the electron if it sits in orbital A.) The wavefunction of the electron can be expressed as

$$|\psi\rangle = c_A\,|A\rangle + c_B\,|A\rangle + c_C\,|C\rangle + c_D\,|D\rangle$$

or as a 4-component vector

$$|\psi\rangle = \begin{pmatrix} c_A \\ c_B \\ c_C \\ c_D \end{pmatrix}$$

The index is again discrete. (It has to be, as the Hilbert space is finite-dimensional.) So the interpretation is in terms of probabilities. Probability densities do not appear. For example $|c_B|^2$ is the probability of finding the electron in orbital B.

3.2 Infinite Hilbert space – continuous index

Consider a particle on a line. Its wavefunction expressed in position basis is the complex function $\psi(x)$. This is a function of a continuous variable x. The index of wavefunction components is continuous. So the interpretation involves **probability densities**. The probability density of the position of the particle is $|\psi(x)|^2$. The probability of finding the particle in the interval between $x = a$ and $x = b$ is

$$\int_a^b dx|\psi(x)|^2$$

> Informally, you could also say that $|\psi(x)|^2 dx$ represents the probability of finding the particle in the interval $(x, x + dx)$, or in the interval $(x - \frac{1}{2}dx, x + \frac{1}{2}dx)$. Either is fine because dx is understood to be infinitesimal, so the value of $|\psi(x)|^2$ is assumed to have negligible variance within these intervals.

Imagine you expressed your wavefunction as a function of momentum, and wrote it as $\tilde{\psi}(p)$. You can obtain $\tilde{\psi}$ by Fourier transforming ψ. As momentum is a continuous variable, you have another situation with a continuous index. So the interpretation of wavefunction components is again as a probability density. The quantity $|\tilde{\psi}(p)|^2 dp$ is the probability of finding the momentum of the particle to be in the range $(p, p + dp)$.

3.3 Infinite Hilbert space – discrete index

Let us represent the eigenfunctions of a harmonic oscillator as

$$|\phi_n\rangle \qquad n = 0, 1, 2, 3, \ldots$$

As you know, they have energy $E_n = (n + 1)\hbar\omega$, where ω is the trapping frequency of the harmonic oscillator.

These eigenstates form a complete basis. The basis has an infinite number of elements in it. This is not surprising, because the Hilbert space of a particle on a continuous line is infinite-dimensional.

As $\{|\phi_n\rangle\}$ is a complete basis, any wavefunction of a single particle on a line can be expressed in terms of these basis states:

$$|\psi\rangle = c_0 |\phi_0\rangle + c_1 |\phi_1\rangle + c_2 |\phi_2\rangle + \ldots = \sum_{n=0}^{\infty} c_n |\phi_n\rangle$$

You can also think of this as an infinite-dimensional vector. Although it's not possible to write out the entire vector, we can make a start:

$$|\psi\rangle = \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ \vdots \\ \vdots \end{pmatrix}$$

The index is **discrete**. So, the interpretation of the components c_n is in terms of discrete probabilities, not probability densities. For example, $|c_3|^2$ is the probability of finding the energy of the particle to be $(3 + \frac{1}{2})\hbar\omega$.

Your particle could be subject to no potential or a completely different potential. Even if your particle is not subject to a harmonic potential, you could expand its wavefunction in terms of the eigenstates of a harmonic oscillator. The essential point is that the harmonic oscillator eigenstates form a complete basis for the complete Hilbert space of any particle on a line.

4 Probability amplitudes

There is a Wikipedia page titled 'Probability amplitude'. It looks quite accessible.

The phrase **probability amplitude** is used to describe any wavefunction component, i.e., a quantity which has to be absolute-squared to obtain a probability or a probability density. Thus, for one of our discrete cases, c_n would be a probability amplitude, and $|c_n|^2$ is a probability. For the continuous case, $\psi(x)$ is a probability amplitude, while $|\psi(x)|^2$ is a probability density.

I don't know the origin of the word 'amplitude' used in this sense. The word means other things in other contexts, for example, the amplitude of a sinusoidal wave is its maximum magnitude. I hope this does not cause too much confusion.