Wavefunctions: Position and Momentum

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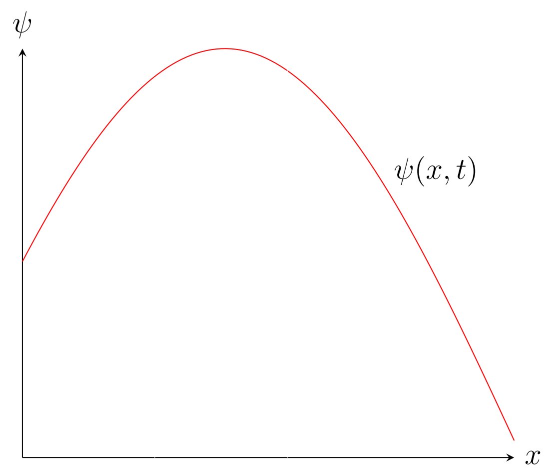
0 Preface

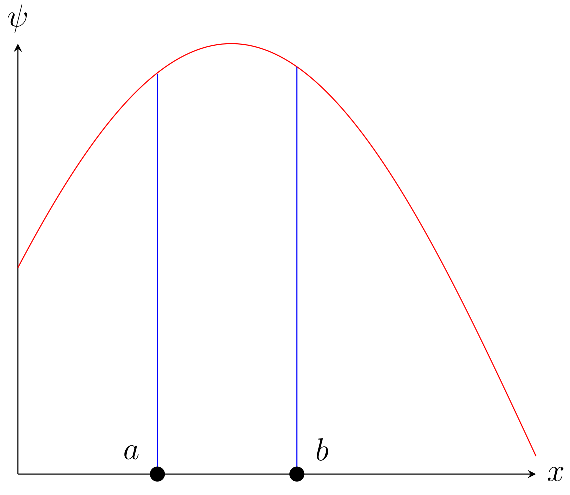
The following notes are based on the lecture video **Position and Momentum from Wavefunctions** (Khan, 2018). The author simply wishes to compile a part of his learning journey into this document.

1 Position

Suppose a particle is described by its wavefunction $\psi(x, t)$.



1.1 Probability of Finding the Position of a Particle



The probability that we will find the particle between two points a and b, is given by the integral:

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

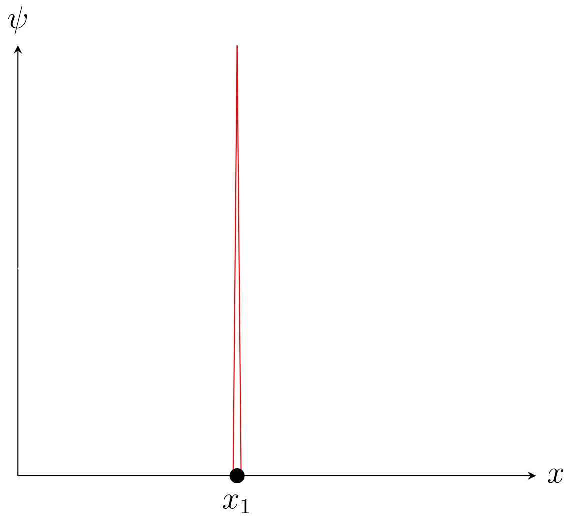
1.2 Expectation Value of the Position of a Particle

While the expectation value of the position is given by the integral:

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi(x,t)|^2 dx \tag{1}$$

What the expectation value represents is **not** the mean value of position from taking several consecutive measurements of the particle.

This is because consecutive measurements would cause **wavefunction collapse**, turning the wavefunction into a delta-function-like graph.



Instead, the expectation value represents the mean value of position from single measurements of an infinite collection of **identical** particles/wavefunctions/systems, at an exact same time.

Alternatively, we can measure one wavefunction, let the system **recover from the collapse**, take the measurement again, repeat, and then finally take the mean of the position.

Both of these methods allow us to calculate the expectation value as:

$$\langle x \rangle = \frac{x_1 + x_2 + .. + x_n}{n}$$

where n is the number of measurements we took.

1.3 Position Operator

Now we'd like to find the corresponding position operator $\hat{x}$, which would be a Hermitian Operator due to the 2^{nd} postulate of Quantum Mechanics.

Recall that the expectation value of the position x can be related to its operator $\hat{x}$ and is defined by the following:

$$\langle x \rangle = \frac{\langle \psi | \hat{x} | \psi \rangle}{\langle \psi | \psi \rangle} \tag{2}$$

We can then equate (1) to (2) since they both represent the expectation value of x:

$$\frac{\langle \psi | \hat{x} | \psi \rangle}{\langle \psi | \psi \rangle} = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$$

Since the wavefunction is normalized, its inner product with itself is 1:

$$\langle \psi | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} x |\psi(x,t)|^2 dx$$

We also know that the magnitude squared of the wavefunction $|\psi|^2$ is just ψ multiplied by its conjugate ψ^*. Substituting that and rearranging the right-hand side yields:

$$\langle \psi | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x) \psi dx$$

From here, we can deduce that the operator $\hat{x}$ is simply given by its position x:

$$\hat{x} = x$$

2 Momentum

Similarly, the momentum of a particle can be represented by a Hermitian Operator $\hat{p}_x$.

We can arrive at this operator by firstly finding the expectation value of its momentum, $\langle p_x \rangle$.

2.1 Expectation Value of the Momentum of a Particle

Surely enough, we can actually derive $\langle p_x \rangle$ using the expectation value of its position $\langle x \rangle$.

We begin by differentiating $\langle x \rangle$ with respect to time:

$$\frac{d\langle x \rangle}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} x|\psi(x,t)|^2 dx$$

$$= \int_{-\infty}^{\infty} \frac{\partial}{\partial t}[x|\psi(x,t)|^2]dx$$

$$= \int_{-\infty}^{\infty} x\frac{\partial}{\partial t}[|\psi(x,t)|^2]dx$$

$$= \int_{-\infty}^{\infty} x\frac{\partial}{\partial t}(\psi^* \cdot \psi)dx$$

Recall that in the derivation of Schrödinger's Equation, we had already found an expression for $\frac{\partial}{\partial t}(\psi^* \cdot \psi)$, plugging that in yields:

$$\frac{d\langle x \rangle}{dt} = \int_{-\infty}^{\infty} x\left[\psi^*\left(\frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2}\right) - \psi\left(\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2}\right)\right]dx$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\left[\psi^*\frac{\partial^2 \psi}{\partial x^2} - \psi\frac{\partial^2 \psi^*}{\partial x^2}\right]dx$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\frac{\partial}{\partial x}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)dx$$

Next, we're going to utilize integration by parts. If we let $u = x$:

$$u = x$$
$$du = \frac{\partial x}{\partial x}$$
$$du = 1$$

and $dv = \frac{\partial}{\partial x}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)$:

$$dv = \frac{\partial}{\partial x}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)$$

$$v = \int_{-\infty}^{\infty} \frac{\partial}{\partial x}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)dx$$

$$v = \psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}$$

Plugging these expressions back to our original integral:

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\left[x\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)dx\right]$$

Because of normalization condition, $\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)\Big|_{-\infty}^{\infty}$ tends to zero, thus:

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right)dx$$

We are going to utilize integration by parts one more time, but only on the right half of the integral:

$$\int_{-\infty}^{\infty}\psi\frac{\partial\psi^*}{\partial x}dx = \psi(\psi^*)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx$$

Again, because of the normalization condition, both ψ and ψ^* tends to zero as x approaches $\pm\infty$. Therefore we are left with:

$$\int_{-\infty}^{\infty}\psi\frac{\partial\psi^*}{\partial x}dx = -\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx$$

Plugging it to the original integral:

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left[\psi^*\frac{\partial\psi}{\partial x} - \left(-\psi^*\frac{\partial\psi}{\partial x}\right)\right]dx$$

$$= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}2\cdot\psi^*\frac{\partial\psi}{\partial x}dx$$

The 2s cancels each other, and we are left with

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx \tag{3}$$

Now, to move forward, we know the postulate that the derivative of the expectation value $\langle x\rangle$ with respect to time is just the expectation value of the velocity operator v_x:

$$\langle v_x\rangle = \frac{d\langle x\rangle}{dt}$$

And the expectation value of the momentum operator $\langle p_x\rangle$ can be related to $\langle v_x\rangle$ by:

$$\langle p_x\rangle = m\langle v_x\rangle$$

Substituting $\langle v_x\rangle$ with the derivative in (3):

$$\langle p_x\rangle = m\left(-\frac{i\hbar}{m}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx\right)$$

$$= -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx$$

Changing the constants in front of the integral into its fraction form yields:

$$\langle p_x\rangle = \frac{\hbar}{i}\int_{-\infty}^{\infty}\psi^*\frac{\partial\psi}{\partial x}dx \tag{4}$$

2.2 Momentum Operator

Similar to finding the position operator, we can start by first representing $\langle p_x \rangle$ in terms of the operator $\hat{p}_x$:

$$\langle p_x \rangle = \frac{\langle \psi | \hat{p}_x | \psi \rangle}{\langle \psi | \psi \rangle} \tag{5}$$

Then equate (4) to (5) since they both are equivalent to $\langle p_x \rangle$:

$$\frac{\langle \psi | \hat{p}_x | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\hbar}{i} \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

The denominator of the left hand side is just 1, and rearranging the right-hand side yields:

$$\langle \psi | \hat{p}_x | \psi \rangle = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi dx$$

From which we can finally deduce the momentum operator $\hat{p}_x$ as:

$$\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

3 Importance of Position and Momentum Operators

Almost all Classical Mechanics quantities can be expressed in terms of position and momentum.

For instance the Kinetic Energy:

$$E_k = \frac{1}{2} m v^2 = \frac{p^2}{2m}$$

and others like the Potential Energy, Angular Momentum, etc.

In general we can find the expectation value of almost any Classical Mechanics quantity Q by using the operators $\hat{x}$ and $\hat{p}_x$:

$$\langle Q(x,p) \rangle = \int_{-\infty}^{\infty} \psi^* Q(\hat{x}, \hat{p}_x) \psi dx$$

References

Khan. (2018). *Position and momentum from wavefunctions — quantum mechanics.* Retrieved from `https://youtu.be/Egu4i8umpoM`