1 Quantization of Light and Matter

Previous Notes

Why bother building 'quantum mechanics' as a framework?

In the first note, we looked at a series of experiments and phenomena to motivate why we would need a quantum mechanical framework and how classical mechanics left us without enough concepts to describe the world we live in.
For material on this section, please refer: Note 1 | Why QM

Quantum Mechanics

In the second note, we introduced some of the postulates of Quantum Mechanics using the Stern-Gerlach experiment as an example that shows inherently *quantum* behaviour.
For material on this section, please refer: Note 2 | QM Framework + Stern Gerlach Experiment

Supplementary Note 1: Mathematical Interlude: *The Wavefunction*

After being exposed to the need for Quantum Mechanics and being introduced to some of its basic postulates, we now improve our mathematical tool-kit. We introduce the notion of a wavefunction, and provide an illustration of the uncertainty principle, which was derived in a rather abstract fashion in the previous note.

Key Takeaway: A brief introduction to the notion of a wavefunction. The main goal is to develop a level of comfort with computations that might usually arise while doing QM.

2 A Mathematical Interlude: The Wavefunction

In this section, we introduce a couple of ideas that would be useful in various parts in the course and contains a number of exercises. The reader is encouraged to work through the exercises.

2.1 Infinite Vector Spaces

Key Concepts: Continuous Basis, Dirac Delta Function, Completeness.

Let us look back at the way we carried out a measurement in the Stern-Gerlach experiment: we let the beam of silver atoms pass through an inhomogeneous magnetic field and observed the direction of deflection. The interesting part is to look at what happens when we allow the deflected silver atoms to deposit on a glass plate. In this case, when a particular atom is deposited on the plate, we get two pieces of information: *what* deflection that atom underwent (spin), and *where* on the plate it ended up (position).

A "position measurement" can yield any value x along the screen. Thus, we need an infinite number of basis kets $\{|x\rangle\}$ to span the space, corresponding to every possible position eigenvalue x. This motivates the need to introduce infinite-dimensional vector spaces.[1]

$$\hat{x}\,|x'\rangle = x'\,|x'\rangle \tag{1}$$

where x' is a real number.

Since the index x is continuous, the discrete sum for orthogonality and completeness would no longer make sense (since it would sum up to infinity!) and instead, an integral is used.

$$\sum \rightarrow \int dx$$

Note that the integral is taken over all space unless specified otherwise.

- **Orthogonality:** Instead of $\langle i|j\rangle = \delta_{ij}$, we have:

  $$\langle x|x'\rangle = \delta(x - x') \tag{2}$$

  where $\delta(x - x')$ is the **Dirac Delta Function**. It is zero everywhere except at $x = x'$, where it is infinite, such that $\int \delta(x)dx = 1$.

- **Completeness:** Instead of $\sum |i\rangle\langle i| = \mathbb{1}$, we have:

  $$\int_{-\infty}^{\infty} dx\,|x\rangle\langle x| = I \tag{3}$$

Exercise: Show that for any state $|\psi\rangle$,

$$|\psi\rangle = \int dx\,\langle x|\psi\rangle\,|x\rangle$$

.

Hint: Remember an idea used in the previous note: $|\psi\rangle = \mathbb{1}\,|\psi\rangle$ *and the completeness relation from above.* (*Key Concept: Function Spaces*)

Since the eigenvectors of a Hermitian operator span the space they live in, the above expression shows how you can expand the state ket in terms of position basis functions.

[1] We do not treat this topic with sufficient rigour. The enthusiastic reader is encouraged to make use of the wonderful notes by Dexter Chua.
Dexter Chua | Linear Algebra
Dexter Chua | Linear Analysis

2.1.1 Wavefunctions

The "coefficient" $\langle x|\psi\rangle$ is a complex-valued function of position. (In analogy with $c_i = \langle a_i|\psi\rangle$ in $|\psi\rangle = \sum_i |a_i\rangle \langle a_i|\psi\rangle$ in the finite dimensional case.) We call this the **Wavefunction**, denoted $\psi(x)$.

$$\psi(x) \equiv \langle x|\psi\rangle \tag{4}$$

Remember the Born Rule: the probability associated with an outcome a with corresponding state $|a\rangle$ is given by $|\langle a|\psi\rangle|^2$. The probability of finding a particle in a small region dx around x is:

$$\begin{aligned} P(x)dx &= |\langle x|\psi\rangle|^2 dx \qquad (5)\\ &= |\psi(x)|^2 dx \qquad (6) \end{aligned}$$

The normalization condition:

$$\begin{aligned} \langle\psi|\psi\rangle &= \langle\psi|\mathbb{1}\psi]\rangle \\ &= \langle\psi| \int |x\rangle \langle x|\, dx|\psi\rangle \\ &= \int \langle\psi|x\rangle \langle x|\psi\rangle\, dx \\ &= \int \psi(x)^*\psi(x)dx \\ &= \int |\psi(x)|^2 dx \\ &= 1 \end{aligned}$$

that is,

$$\int |\psi(x)|^2 dx = 1 \tag{7}$$

2.1.2 Momentum Space

Instead of position, we could alternatively express the state in terms of the *momentum basis* $|p\rangle$.

$$\phi(p) \equiv \langle p|\psi\rangle \tag{8}$$

How do we relate $\psi(x)$ and $\phi(p)$? We know:

$$\begin{aligned} \langle x|\psi\rangle &= \langle x|\mathbb{1}|\psi\rangle \\ &= \langle x| \int |p\rangle \langle p|\, \psi\rangle\, dp \\ &= \int \langle x|p\rangle \langle p|\psi\rangle\, dp \end{aligned}$$

$$\langle p|\psi\rangle = \int \langle p|x\rangle\, \psi(x)dx \tag{9}$$

We need the inner product $\langle x|p\rangle$. Motivated by de Broglie's relation ($p = \hbar k$) and plane waves (e^{ikx}), we postulate

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{10}$$

We will return to a strict derivation of this relation using *Translation Operators* when we do time-evolution in the next note[2]

[2]The enthusiastic reader is referred to section 1.7 of Sakurai & Napolitano (2011).

Using the completeness relation:

$$\langle x|\psi\rangle = \int dp\, \langle x|p\rangle \langle p|\psi\rangle \tag{11}$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp e^{ipx/\hbar} \phi(p) \tag{12}$$

This is exactly a **Fourier Transform**! The position and momentum space wavefunctions are Fourier transforms of each other.

Exercise: We showed that by taking the Fourier Transform of $\phi(p)$ we get $\psi(x)$. How do you get $\phi(p)$ from $\psi(x)$. Derive the relation and show that the inverse Fourier Transform is exactly what you need! *Hint: Use the completeness relation just like we did above.*

2.1.3 Position and Momentum Operators

In the position basis, the position operator $\hat{x}$ acts simply as multiplication by x:

$$\begin{aligned} \langle x|\hat{x}|\psi\rangle &= x^* \langle x|\psi\rangle && (\text{using } \hat{x}|x\rangle = x|x\rangle) && (23)\\ &= x\psi(x) && (\text{position is real, } x = x^*) && (24) \end{aligned}$$

However, the momentum operator $\hat{p}$ must generate translations (move the function). In the position representation, it takes the form of a derivative[3]:

$$\hat{p} \equiv -i\hbar \frac{\partial}{\partial x} \tag{13}$$

Exercise: Check that $[\hat{x}, \hat{p}]\psi(x) = i\hbar\psi(x)$.
Hint:

$$[\hat{x}, \hat{p}]\psi(x) = x(-i\hbar\frac{\partial}{\partial x})\psi(x) - (-i\hbar\frac{\partial}{\partial x})(x\psi(x))$$

Thus $[\hat{x}, \hat{p}] = i\hbar\mathbb{1}$. This non-zero commutator confirms that x and p cannot be simultaneously measured with arbitrary precision, from the Uncertainty Principle introduced in the previous note.

To recall:

$$\Delta(x)\Delta(p) \geq \frac{|\langle\psi|[x, p]|\psi\rangle|}{2}. \tag{14}$$

Exercise: Verify the above relation. *Hint:*
Remember:

$$\begin{aligned} \langle x\rangle &= \langle\psi|\hat{x}|\psi\rangle \\ \langle x^2\rangle &= \langle\psi|\hat{x}^2|\psi\rangle \\ &= \langle\psi|\hat{x}\hat{x}|\psi\rangle \\ \Delta x &= \sqrt{\langle x^2\rangle - \langle x\rangle^2} \end{aligned}$$

2.2 Illustrating the Uncertainty Principle

Exercise: Compute the momentum space representation for the following wavefunction

$$\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{15}$$

[3]We will derive this as well at a later stage when we do the Translation operator.

And verify that $\phi(p)$ is also a Gaussian!

The Fourier transform relationship implies that if $\psi(x)$ is very localized (narrow peak), its Fourier transform $\phi(p)$ must be very spread out (wide), and vice versa. Remember that we met the Uncertainty Principle in the previous note:

Let's visualize this with a Gaussian wavepacket.

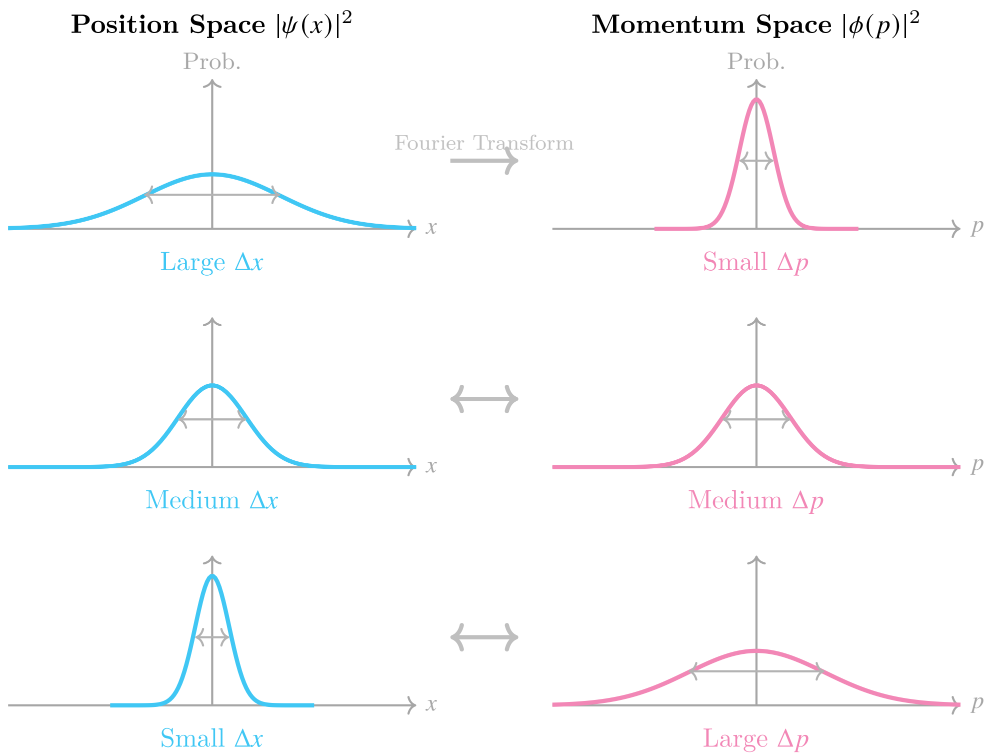

Figure 1: Visualizing the Uncertainty Principle with normalized Gaussian wavepackets. The probability density curves in position space (light blue) and momentum space (light red) are related by Fourier transform. As the position distribution becomes narrower (top to bottom), the peak height increases to conserve probability. Simultaneously, the corresponding momentum distribution becomes wider and shorter, illustrating the inverse relationship between Δx and Δp.

Summary: Infinite Dimensions & Wavefunctions

In this section, we generalized the vector space formalism to **infinite dimensions** to describe continuous variables like position.

- **Continuous Basis:** Discrete sums are replaced by integrals ($\sum \to \int$), and the Kronecker delta is replaced by the **Dirac Delta function**, $\delta(x - x')$.
- **Wavefunctions:** The coefficient of the state in the position basis, $\psi(x) = \langle x|\psi\rangle$, is the wavefunction. The probability density is given by $|\psi(x)|^2$.
- **Momentum Space:** The momentum representation $\phi(p)$ is the **Fourier Transform** of the position wavefunction. This mathematical relationship dictates that localizing a particle in position spreads it out in momentum (and vice versa).
- **Operators:** In position space, $\hat{x}$ acts as a multiplier x, while $\hat{p}$ acts as the derivative $-i\hbar\frac{\partial}{\partial x}$. Their non-zero commutator $[\hat{x}, \hat{p}] = i\hbar$ leads directly to the Heisenberg Uncertainty Principle.

In-Chapter Visualization

We numerically illustrate the Gaussian wavefunction, its Fourier transform, and the uncertainty principle.
Run the interactive notebook here: Gaussian Uncertainty Notebook

References

J. J. Sakurai and Jim Napolitano. *Modern Quantum Mechanics*. Addison-Wesley, San Francisco, CA, 2nd edition, 2011. ISBN 978-0-8053-8291-4.