Lecture notes: QM 04

Expectation values of operators

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Contents

1 Momentum space

We begin with Fourier transformation to make a series of developments that lead to the idea of momentum space as a counterpoint or dual of position space. In this section the time dependence of wave functions will play no role. Therefore we will simply suppress time dependence. You can imagine all wave functions evaluated at time equal zero or at some arbitrary time t_0.

A wave packet is a superposition of plane waves e^{ikx} with various wavelengths. According to Fourier's theorem such a wave packet have the form

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} \, \mathrm{d}k. \tag{1}$$

The function $\Phi(k)$ acts as the weight with which we add the plane waves with momentum $\hbar k$ to form $\Psi(x)$. Thus the Fourier representation of the wave $\Psi(x)$ gives the way to represent the wave as a superposition of plane waves of different momenta. If we know $\Psi(x)$ then $\Phi(k)$ is calculable. In fact, by the Fourier inversion theorem, the function $\Phi(k)$ is the Fourier transform of $\Psi(x)$, so we can write

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx} \, \mathrm{d}x. \tag{2}$$

Note the symmetry in the two equations above. The Fourier transform $\Phi(k)$ has all the information carried by the wave function $\Psi(x)$. This is clear because knowing $\Phi(k)$ means knowing $\Psi(x)$.

The consistency of the above equations can be used to derive an integral representation for a delta function. The idea is to replace $\Phi(k)$ in (1) by the value given in (2). In order to keep the notation clear, we must use x' as a dummy variable of integration in the second equation. We have

$$\begin{aligned}\Psi(x) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ikx}\, \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x'\, e^{-ikx'}\Psi(x') \\ &= \int_{-\infty}^{\infty} \mathrm{d}x'\, \Psi(x')\, \underbrace{\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x-x')}} . \end{aligned} \tag{3}$$

The factor indicated by the brace happens to reduce the x' integral to an evaluation at x. We know that $\delta(x'-x)$ is the function such that for general $f(x)$

$$\int_{-\infty}^{\infty} \mathrm{d}x'\, f(x')\, \delta(x'-x) = f(x) \tag{4}$$

and so we conclude that the factor indicated by the brace is a delta function

$$\delta(x'-x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x-x')}. \tag{5}$$

In this integral one can let $k \to -k$ and since $\int \mathrm{d}k$ is left invariant under this replacement, we find that $\delta(x'-x) = \delta(x-x')$, or more plainly $\delta(x) = \delta(-x)$. We will record the integral representation of the delta function using the other sign:

$$\boxed{\delta(x-x') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{ik(x-x')}.} \tag{6}$$

Another useful property of delta functions is

$$\delta(ax) = \frac{1}{|a|}\delta(x). \tag{7}$$

To understand how the normalization condition for $\Psi(x)$ look like in terms of $\Phi(k)$, we calculate

$$\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \Phi^*(k)e^{-ikx}\,\mathrm{d}k\, \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \Phi(k')e^{ik'x}\,\mathrm{d}k'. \tag{8}$$

Rearranging the integrals to do the x integral first we write

$$\begin{aligned}\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)\,\mathrm{d}x &= \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}k'\, \Phi^*(k)\Phi(k')\, \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(k'-k)x}\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty} \mathrm{d}k \int_{-\infty}^{\infty} \mathrm{d}k'\, \Phi^*(k)\Phi(k')\, \delta(k'-k) \\ &= \int_{-\infty}^{\infty} \mathrm{d}k\, \Phi^*(k)\Phi(k'), \end{aligned} \tag{9}$$

where we recognized the presence of a delta function and we did the integral over k'. Our final result is therefore

$$\boxed{\int_{-\infty}^{\infty} |\Psi(x)|^2 \mathrm{d}x = \int_{-\infty}^{\infty} |\Phi(k)|^2 \mathrm{d}k.} \tag{10}$$

This is known as Parseval's theorem, or more generally, Plancherel's theorem. This equation relates the $\Psi(x)$ normalization to a rather analogous normalization for $\Phi(k)$. This is a hint that just like for $|\Psi(x)|^2$, we may have a probability interpretation for $|\Phi(k)|^2$.

Since physically we associate our plane waves with eigenstates of momentum, let us rewrite Parseval's theorem using momentum $p = \hbar k$. Instead of integrals over k we will have integrals over p. With $\widetilde{\Phi}(p) = \Phi(k)$ equations (1) and (2) can be rewritten as

$$\begin{aligned} \Psi(x) &= \frac{1}{\sqrt{2\pi}\,\hbar} \int_{-\infty}^{\infty} \widetilde{\Phi}(p)\, e^{ipx/h}\, \mathrm{d}p, \\ \widetilde{\Phi}(p) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x)\, e^{-ipx/h}\, \mathrm{d}x. \end{aligned} \tag{11}$$

For a more symmetric pair of equations we can redefine the function $\widetilde{\Phi}(p)$. We let $\widetilde{\Phi}(p) \to \Phi(p)\sqrt{\hbar}$ in (11) to obtain our final form for Fourier's relations in terms of momentum:

$$\boxed{\begin{aligned} \Psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p)\, e^{ipx/h}\, \mathrm{d}p, \\ \Phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x)\, e^{-ipx/h}\, \mathrm{d}x. \end{aligned}} \tag{12}$$

Similarly, Parseval's theorem (10) becomes

$$\boxed{\int_{-\infty}^{\infty} |\Psi(x)|^2 \mathrm{d}x = \int_{-\infty}^{\infty} |\Phi(p)|^2 \mathrm{d}p.} \tag{13}$$

Our interpretation of the top equation in (12) is that $\Phi(p)$ denotes the weight with which we add the momentum state $e^{ipx/\hbar}$ in the superposition that represents $\Psi(x)$. This momentum state $e^{ipx/\hbar}$ is an eigenstate of the momentum operator $\hat{p}$ with eigenvalue p. Just like we say that $\Psi(x)$ is the wave function in position space x, we can think of $\Phi(p)$ as the wave function in momentum space p. The Parseval identity (13) suggests that $\Phi(p)$ has a probabilistic interpretation as well. Given that a properly normalized $\Psi(x)$ leads to a $\Phi(p)$ that satisfies

$$\int_{-\infty}^{\infty} |\Phi(p)|^2 \mathrm{d}p = 1, \tag{14}$$

we postulate that:

$|\Phi(p)|^2 \mathrm{d}p$ is the probability to find the particle with momentum in the range $[p,\, p+\mathrm{d}p]$.

This makes the analogy between position and momentum space quite complete.

Fourier's theorem in momentum space language for three dimension takes the form

$$\boxed{\begin{aligned} \Psi(\mathbf{r}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \Phi(\mathbf{p})\, e^{i\mathbf{p}\cdot\mathbf{r}/h}\, \mathrm{d}\mathbf{p}, \\ \Phi(\mathbf{p}) &= \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \Psi(\mathbf{r})\, e^{-i\mathbf{p}\cdot\mathbf{r}/h}\, \mathrm{d}\mathbf{r}. \end{aligned}} \tag{15}$$

Just like one dimensional case using the definition of three dimensional delta function

$$\delta^3(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \tag{16}$$

one can arrive to Parseval's identity:

$$\boxed{\int_{-\infty}^{\infty} |\Psi(\mathbf{r})|^2 \mathrm{d}\mathbf{r} = \int_{-\infty}^{\infty} |\Phi(\mathbf{p})|^2 \mathrm{d}\mathbf{p},} \tag{17}$$

where $|\Phi(\mathbf{p})|^2 \mathrm{d}\mathbf{p}$ is the probability to find the particle with momentum in the range $\mathrm{d}\mathbf{p}$ around $\mathbf{p}$.

2 Expectation values of operators

Consider a random variable ω that takes values in the set $\{\Omega_1, \ldots, \Omega_n\}$ with respective probabilities $\{p_1, \ldots, p_n\}$. The *expectation value* $\langle\Omega\rangle$ (or *expected value*) of Ω is the average value that we expect to find after repeated observation of Ω, and is given by the formula

$$\langle\Omega\rangle = \sum_{i=1}^{n} p_i\, \Omega_i. \tag{18}$$

In quantum system the probability for a particle to be found in $[x, x+\mathrm{d}x]$ at time t is given by $\Psi^*(x,t)\Psi(x,t)\,\mathrm{d}x$. Thus, the expectation value of x, denoted as $\langle x\rangle$ is given by

$$\langle x\rangle \equiv \int_{-\infty}^{\infty} x\, \Psi^*(x,t)\Psi(x,t)\, \mathrm{d}x. \tag{19}$$

The physical meaning of this would be if we consider many copies of the identical system, and measure the position x at a time t in all of them, then the average value recorded will converge to $\langle x\rangle$ as the number of systems and measurements approaches infinity. Note that the expectation depends on time t.

Let us now discuss the expectation value for the momentum. Since $\Phi^*(p,t)\Phi(p,t)\,\mathrm{d}p$ is the probability of finding the particle with momentum in the range $[p,\,p+\mathrm{d}p]$ at time t, we define the expectation value of the momentum as

$$\langle p\rangle \equiv \int_{-\infty}^{\infty} p\,\Phi^*(p,t)\Phi(p,t)\,\mathrm{d}p. \tag{20}$$

We will now manipulate this expression to see what form it takes in coordinate space. Using (12) and its complex conjugate version we have

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} p\,\Phi^*(p,t)\Phi(p,t)\,\mathrm{d}p \\
&= \int_{-\infty}^{\infty} \mathrm{d}p\,p \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi\hbar}}\Psi^*(x,t)\,e^{ipx/\hbar} \int_{-\infty}^{\infty} \frac{\mathrm{d}x'}{\sqrt{2\pi\hbar}}\Psi(x',t)\,e^{-ipx'/\hbar} \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}x\,\Psi^*(x,t)\int_{-\infty}^{\infty} \mathrm{d}x'\,\Psi(x',t)\int_{-\infty}^{\infty} \mathrm{d}p\,p\,e^{ipx/\hbar}\,e^{-ipx'/\hbar} \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}x\,\Psi^*(x,t)\int_{-\infty}^{\infty} \mathrm{d}x'\,\Psi(x',t)\int_{-\infty}^{\infty} \mathrm{d}p\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)e^{ipx/\hbar}\,e^{-ipx'/\hbar} \\
&= \int_{-\infty}^{\infty} \mathrm{d}x\,\Psi^*(x,t)\int_{-\infty}^{\infty} \mathrm{d}x'\,\Psi(x',t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}p\,e^{ipx/\hbar}\,e^{-ipx'/\hbar}.
\end{aligned} \tag{21}$$

Using $p=\hbar u$ in the final integral we have

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}p\,e^{ipx/\hbar}\,e^{-ipx'/\hbar} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}u\,e^{iu(x-x')} = \delta(x-x'). \tag{22}$$

As a result, we have

$$\begin{aligned}
\langle p\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\,\Psi^*(x,t)\int_{-\infty}^{\infty} \mathrm{d}x'\,\Psi(x',t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\delta(x-x') \\
&= \int_{-\infty}^{\infty} \mathrm{d}x\,\Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\int_{-\infty}^{\infty} \mathrm{d}x'\,\Psi(x',t)\delta(x-x') \\
&= \int_{-\infty}^{\infty} \mathrm{d}x\,\Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi(x,t).
\end{aligned} \tag{23}$$

Finally with $\hat{p} = -i\hbar\dfrac{\partial}{\partial x} = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$ we have shown that

$$\boxed{\langle p\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\,\hat{p}\Psi(x,t)\,\mathrm{d}x.} \tag{24}$$

Notice the position of the $\hat{p}$ operator: it acts on $\Psi(x,t)$. This motivates the following definition for the expectation value $\langle\Omega\rangle$ of any operator $\hat{\Omega}$:

$$\boxed{\langle\Omega\rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\,\hat{\Omega}\Psi(x,t)\,\mathrm{d}x.} \tag{25}$$

Example: Consider the kinetic energy operator $\hat{T}$ for a particle moving in 1D:

$$\hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \tag{26}$$

According to the definition (25) we have

$$\begin{aligned}\langle T\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(x,t)\, \hat{T}\Psi(x,t) \\ &= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \mathrm{d}x\, \Psi^*(x,t)\, \frac{\partial^2}{\partial x^2}\Psi(x,t). \end{aligned} \tag{27}$$

The kinetic energy is a positive operator (being proportional to the square of the momentum operator). It is therefore of interest to make this positivity manifest. Integrating by parts one of the x derivatives and ignoring boundary terms that are presumed to vanish, we find

$$\langle T\rangle = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} \left|\frac{\partial\Psi(x,t)}{\partial x}\right|^2 \mathrm{d}x. \tag{28}$$

This is manifestly positive! The expectation value of T can also be computed in momentum space using the probabilistic interpretation that led to (20):

$$\langle T\rangle = \int_{-\infty}^{\infty} \frac{p^2}{2m}|\Phi(p,t)|^2\, \mathrm{d}p. \tag{29}$$

3 Uncertainty

For random variables, the uncertainty is the standard deviation i.e. the square root of the expected value of the square of deviations from the average value. Let Ω be a random variable that takes on values $\{\Omega_1,\ldots,\Omega_n\}$ with probabilities $\{p_1,\ldots,p_n\}$, respectively. The expectation value is

$$\overline{\Omega} = \sum_i p_i\, \Omega_i, \tag{30}$$

and the variance (the square of the standard deviation) is

$$(\Delta\Omega)^2 \equiv \sum_i p_i(\Omega_i - \Delta\Omega)^2. \tag{31}$$

This definition makes it clear that if $\Delta\Omega = 0$, then the random variable is constant: each term in the above sum must vanish, making $\Omega_i = \Delta\Omega$, for all i. We find another useful expression by expanding the above definition

$$\begin{aligned}(\Delta\Omega)^2 &= \sum_i p_i\,\Omega_i^2 - \sum_i p_i\,\Omega_i\overline{\Omega} + \sum_i p_i\overline{\Omega}^2 \\ &= \overline{\Omega^2} - 2\overline{\Omega}\,\overline{\Omega} + \overline{\Omega}^2 \\ &= \overline{\Omega^2} - \overline{\Omega}^2, \end{aligned}\tag{32}$$

where we used $\sum_i p_i = 1$. Since, by definition $(\Delta\Omega)^2 \geq 0$, we have interesting inequality

$$\overline{\Omega^2} \geq \overline{\Omega}^2. \tag{33}$$

Now let us consider the quantum mechanical case. Following (32) we declare that the square of the uncertainty $\Delta\Omega$ of a variable is a real number whose square is given by

$$\boxed{(\Delta\Omega)^2 = \langle\Omega^2\rangle - \langle\Omega\rangle^2.} \tag{34}$$

Hence the uncertainty is given as

$$\boxed{\Delta\Omega = \sqrt{\langle\Omega^2\rangle - \langle\Omega\rangle^2}.} \tag{35}$$

Since the right-hand side of (34) can be written as

$$\langle\Omega^2\rangle - \langle\Omega\rangle^2 = \langle\Omega^2\rangle - 2\langle\Omega\rangle\langle\Omega\rangle + \langle\Omega\rangle^2 = \langle\Omega^2 - 2\Omega\langle\Omega\rangle + \langle\Omega\rangle^2\rangle, \tag{36}$$

the square of uncertainty can also be written as the expectation value of the square of the difference between the operator and its expectation value:

$$(\Delta\Omega)^2 = \langle(\Omega - \langle\Omega\rangle)^2\rangle. \tag{37}$$

4 Time dependence of expectation values

The expectation values of operators are in general time dependent because the wave functions representing the states are time dependent. We will consider here operators that do not have explicit time dependence, that is, operators that do not involve any time derivatives. Taking the time derivative on both sides of (25) and then multiplying with $i\hbar$ we have

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle &= i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}\Psi^*(x,t)\,\hat{\Omega}\Psi(x,t)\,\mathrm{d}x \\ &= i\hbar\int_{-\infty}^{\infty}\left(\frac{\partial\Psi^*}{\partial t}\,\hat{\Omega}\Psi + \Psi^*\,\hat{\Omega}\frac{\partial\Psi}{\partial t}\right)\mathrm{d}x. \end{aligned} \tag{38}$$

Now using the Schrödinger equation $i\hbar\dfrac{\partial\Psi}{\partial t} = \hat{H}\Psi$ and its complete conjugate we have

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle &= \int_{-\infty}^{\infty}\left\{-(\hat{H}\Psi)^*\,\hat{\Omega}\Psi + \Psi^*\,\hat{\Omega}(\hat{H}\Psi)\right\}\mathrm{d}x \\ &= \int_{-\infty}^{\infty}\left\{\Psi^*\,\hat{\Omega}(\hat{H}\Psi) - (\hat{H}\Psi)^*\,\hat{\Omega}\Psi\right\}\mathrm{d}x. \end{aligned} \tag{39}$$

Recall the Hermiticity of $\hat{H}$, which implies that

$$\int_{-\infty}^{\infty}(\hat{H}\Psi_1)^*\,\Psi_2\,\mathrm{d}x = \int_{-\infty}^{\infty}\Psi_1^*\,\hat{H}\Psi_2\,\mathrm{d}x. \tag{40}$$

This can be applied to the second term in the last right-hand side of (39) to move $\hat{H}$ into the other wave function

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle &= \int_{-\infty}^{\infty}(\Psi^*\,\hat{\Omega}\hat{H}\Psi - \Psi^*\,\hat{H}\hat{\Omega}\Psi)\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty}\Psi^*(\hat{\Omega}\hat{H} - \hat{H}\hat{\Omega})\Psi\,\mathrm{d}x \\ &= \int_{-\infty}^{\infty}\Psi^*[\hat{\Omega},\,\hat{H}]\Psi\,\mathrm{d}x, \end{aligned} \tag{41}$$

where we noted the appearance of the commutator. All in all, we have proven that for operators $\hat{\Omega}$ that do not explicitly depend on time,

$$\boxed{i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle = \left\langle[\hat{\Omega},\, \hat{H}]\right\rangle.} \tag{42}$$

Therefore, for an operation which commute with the Hamiltonian operator $\hat{H}$ the expectation value will not change over time. For example for a free particle the Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m}. \tag{43}$$

Hence the momentum operator $\hat{p}$ commute with $\hat{H}$ that is

$$[\hat{p},\, \hat{H}] = [\hat{p},\, \frac{\hat{p}^2}{2m}] = \frac{1}{2m}[\hat{p},\, \hat{p}^2] = \frac{1}{2m}\Big([\hat{p},\, \hat{p}]\hat{p} + \hat{p}[\hat{p},\, \hat{p}]\Big) = 0. \tag{44}$$

This gives us

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = \left\langle[\hat{p},\, \hat{H}]\right\rangle = 0. \tag{45}$$

For a free particle the expectation value of momentum does not change over time i.e. for a free particle the the expectation value of momentum is conserved.

Note: Most of the materials in this lecture note are taken from the Lecture Notes on Quantum Mechanics by Barton Zwiebach given for the course 8.04, 2016 at MIT.

References

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2. Introduction to Quantum Mechanics by David J. Griffiths