# Statistical Interpretation

Lecture 15

Physics 342
Quantum Mechanics I

Friday, February 29th, 2008

Quantum mechanics is a theory of probability densities – given that we now have an abstract vector space in which the (square root of the) probability density lives, we need to translate our usual ideas about probabilities into the Bra-ket language. We can expand our use of the notation, and make some interpretive points as we go.

## 15.1 Averages in Momentum Space

The identification of the expectation value of an operator $A$:

$$\langle A \rangle = \int_{-\infty}^{\infty} \psi(x)^* \, A \, \psi(x) \, dx \tag{15.1}$$

in position basis begs the question: Can we perform the average w.r.t. the momentum basis? Sure, think of the bra-ket representation

$$\langle A \rangle = \langle \Psi | \, A \, | \Psi \rangle = \int_{-\infty}^{\infty} \langle \Psi | p \rangle \, \langle p | \, A \, | \bar{p} \rangle \, \langle \bar{p} | \Psi \rangle \; dp \, d\bar{p} \tag{15.2}$$

obtained by introducing the identity in the form $\int_{-\infty}^{\infty} | p \rangle \langle p | \; dp$ twice. We have, in terms of functions,

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi(p)^* \; \langle p | \, A \, | \bar{p} \rangle \; \Psi(\bar{p}) \, dp \, d\bar{p}. \tag{15.3}$$

In this context, the representation of $A$ is w.r.t. the $p$ basis, and the object $\langle p | \, A \, | \bar{p} \rangle$ is called the "matrix element of $A$ w.r.t. the basis $| p \rangle$"[1]. How do

[1]Think of the analagous finite-dimensional object, which would look like $\mathbf{e}_i^\dagger \, \mathbb{A} \, \mathbf{e}_j = A_{ij}$

we figure out the "matrix elements" for a given operator $A$? Let's work out the form for a particular operator – $x$, for example.

We want $\langle p| x |\bar{p}\rangle$, and expanding using the identity operator, we have

$$\langle p| x |\bar{p}\rangle = \int_{-\infty}^{\infty} \langle p|\bar{x}\rangle \, \langle \bar{x}| x |\hat{x}\rangle \, \langle \hat{x}|\bar{p}\rangle \, d\bar{x}\, d\hat{x}. \tag{15.4}$$

Since $|\hat{x}\rangle$ is an eigenket of the $x$ operator (with eigenvalue $\hat{x}$), we can write $\langle \bar{x}| x |\hat{x}\rangle = \hat{x}\, \langle \bar{x}|\hat{x}\rangle = \hat{x}\, \delta(\bar{x} - \hat{x})$. Using our functional form: $\langle p|\bar{x}\rangle = \frac{1}{\sqrt{2\,\pi\,\hbar}}\, e^{-\frac{i\,p\,\bar{x}}{\hbar}}$, and its conjugate, the integral becomes

$$\begin{aligned}
\langle p| x |\bar{p}\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\,\pi\,\hbar}}\, e^{-\frac{i\,p\,\bar{x}}{\hbar}}\, \hat{x}\, \delta(\bar{x}-\hat{x})\, \frac{1}{\sqrt{2\,\pi\,\hbar}}\, e^{\frac{i\,\hat{x}\,\bar{p}}{\hbar}}\, d\bar{x}\, d\hat{x} \\
&= \frac{1}{2\,\pi\, i}\frac{d}{d\bar{p}} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{i\,p\,\bar{x}}{\hbar}}\, e^{\frac{i\,\hat{x}\,\bar{p}}{\hbar}}\, \delta(\bar{x}-\hat{x})\, d\bar{x}\, d\hat{x} \\
&= \frac{1}{2\,\pi\, i}\, \frac{d}{dp} \int_{-\infty}^{\infty} e^{\frac{i\,\hat{x}\,(\bar{p}-p)}{\hbar}}\, d\hat{x} \\
&= \frac{\hbar}{i}\, \frac{\partial}{\partial \bar{p}}\, \delta(\bar{p}-p).
\end{aligned} \tag{15.5}$$

Now, let's go back to our original object of interest (15.1), in the form (15.3) – let $A = x$, since we just did the relevant computation there:

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{\infty} \langle \Psi|p\rangle \, \langle p| x |\bar{p}\rangle \, \langle \bar{p}|\Psi\rangle \, dp\, d\bar{p} \\
&= \int_{-\infty}^{\infty} \Psi(p)^* \left(\frac{\hbar}{i}\, \frac{d}{d\bar{p}}\, \delta(\bar{p}-p)\right)\, \Psi(\bar{p})\, dp\, d\bar{p} \\
&= \int_{-\infty}^{\infty} \Psi(p)^* \left(-\frac{\hbar}{i}\, \frac{d\Psi(p)}{dp}\right)\, dp,
\end{aligned} \tag{15.6}$$

where we integrate by parts to flip the derivative with respect to $\bar{p}$ from the $\delta$ to the $\Psi(\bar{p})$, then use the $\delta(\bar{p}-p)$ to perform the $\bar{p}$ integration. Evidently, then, the operator $x$ acting in momentum space has the form $-\frac{\hbar}{i}\frac{d}{dp}$, similar to the momentum operator $p$ in position space.

Incidentally, this implies that the Schrödinger equation could be written in momentum space. Perhaps we have more interest in momentum than position, then we can use operators $p$ and $-\frac{\hbar}{i}\frac{\partial}{\partial p}$ to generate Schrödinger's equation from a classical potential $V(x,p)$:

$$\boxed{\frac{p^2}{2\,m}\, \Psi(p,t) + V\left(-\frac{\hbar}{i}\frac{\partial}{\partial p}, p\right)\, \Psi(p,t) = i\,\hbar\, \frac{\partial \Psi(p,t)}{\partial t}.} \tag{15.7}$$

## 15.2 Hermitian Operators

As with their finite brethren, Hermitian operators play a special role in the mathematics of our infinite dimensional function space, and have a physical interpretation that is part of the basic axiomatic development of quantum mechanics. On the matrix side, we call $\mathbb{A}$ Hermitian if $\mathbb{A} = \mathbb{A}^\dagger$, just the complex analogue of symmetric. More to the point, if we have a vector $\mathbf{v}$, then

$$\mathbb{A}\,\mathbf{v} = (\mathbf{v}^\dagger\,\mathbb{A})^\dagger, \tag{15.8}$$

and if we take another arbitrary vector $\mathbf{w}$:

$$\mathbf{w}^\dagger\,\mathbb{A}\,\mathbf{v} = (\mathbb{A}\,\mathbf{w})^\dagger\,\mathbf{v} \tag{15.9}$$

which is not true of any old matrix. The advantage to Hermitian matrices is that they are diagonalized by unitary matrices, ones with $\mathbb{U}^\dagger\,\mathbb{U} = I$ and this just means that the columns of $\mathbb{U}$ form a basis (again the complex generalization of symmetric matrices – these are diagonalized by "orthogonal" matrices with $\mathbb{O}^T\,\mathbb{O} = I$). In addition, the eigenvalues associated with Hermitian matrices are real.

These matrix-vector relations can be generalized in our bra-ket notation. Consider an operator $\hat{A}$ acting on a ket $|v\rangle$: $\hat{A}\ |v\rangle$ and a bra $\langle w|$ via "$\left\langle \hat{A}\,w \right|$". In this language, the (15.9) requirement is, awkwardly[2]:

$$\langle w|\ \hat{A}\ |v\rangle = (\hat{A}\ |w\rangle)^\dagger\ |v\rangle = \left\langle \hat{A}\,w \middle| v \right\rangle. \tag{15.12}$$

This gives the "expectation value" of a Hermitian operator $\hat{A}$ a preferred place in the statistical interpretation – since

$$\langle \hat{A}\rangle = \langle \Psi|\,\hat{A}\,|\Psi\rangle = \left\langle \hat{A}\Psi \middle| \Psi \right\rangle = \langle \hat{A}\rangle^*, \tag{15.13}$$

[2]We can make more sense of this requirement in the position basis:

$$\langle w|\hat{A}|v\rangle = \int_{-\infty}^{\infty} w(x)^*\,\hat{A}\,v(x)\,dx. \tag{15.10}$$

The $\hat{A}$ is Hermitian if:

$$\int_{-\infty}^{\infty} w(x)^*\,\hat{A}\,v(x)\,dx = \int_{-\infty}^{\infty} \left(\hat{A}\,w(x)\right)^*\,v(x)\,dx. \tag{15.11}$$

so that the expectation value is real, just what we would expect from the average of some physical observable.

Establishing that an operator is Hermitian can be done in various ways (meaning, in various bases) – take the position and momentum operators in position space. We have

$$\begin{aligned}\langle\Psi|\, x\, |\Psi\rangle &= \int_{-\infty}^{\infty} \Psi(x,t)^*\, x\, \Psi(x,t)\, dx = \int_{-\infty}^{\infty} (x\, \Psi(x,t))^*\, \Psi(x,t)\, dx \\ &= \langle x\Psi|\Psi\rangle\end{aligned} \tag{15.14}$$

for the position operator, trivially. The momentum operator is more involved,

$$\begin{aligned}\langle\Psi|\, p\, |\Psi\rangle &= \int_{-\infty}^{\infty} \Psi(x,t)^*\, \frac{\hbar}{i}\, \frac{\partial \Psi(x,t)}{\partial x}\, dx \\ &= -\int_{-\infty}^{\infty} \frac{\hbar}{i}\, \frac{\partial \Psi(x,t)^*}{\partial x}\, \Psi(x,t)\, dx \\ &= \int_{-\infty}^{\infty} \left(\frac{\hbar}{i}\, \frac{\partial \Psi(x,t)}{\partial x}\right)^*\, \Psi(x,t)\, dx \\ &= \langle p\, \Psi|\Psi\rangle\, .\end{aligned} \tag{15.15}$$

Powers of Hermitian operators are also Hermitian, if $\hat{A}$ is Hermitian, then so is $\hat{A}\,\hat{A}$, since

$$\langle v|\, \hat{A}\, \hat{A}\, |w\rangle = \left\langle \hat{A}\, v \middle|\, \hat{A}\, |w\right\rangle = \left\langle \hat{A}\, \hat{A}\, v \middle| w\right\rangle, \tag{15.16}$$

and then we see that the Hamiltonian operator, $H = \frac{p^2}{2\,m} + V(x)$ is automatically Hermitian.

Note that it is always possible to construct the "Hermitian conjugate" for an operator, just as we can for matrices – it is defined to be the operator $\hat{A}^\dagger$ such that $\left\langle \hat{A}^\dagger v \middle| w\right\rangle = \langle v|\, A\, |w\rangle$, so the notation $\hat{A} = \hat{A}^\dagger$ makes sense for operators, even though it is not immediately clear how to take the "conjugate transpose" of $\frac{\hbar}{i}\frac{\partial}{\partial x}$.

## 15.3 Commutators and Determinant States

Recall our harmonic oscillator Hamiltonian – we wrote $H = \frac{p^2}{2\,m} + \frac{1}{2}\,m\,\omega^2\,x^2$ in terms of the operators $a_+$ and $a_-$

$$a_\pm \equiv \frac{1}{\sqrt{2\,\hbar\,m\,\omega}}(\mp i\,p + m\,\omega\,x) \qquad H = \hbar\,\omega\left(a_\pm\,a_\mp \pm \frac{1}{2}\right). \tag{15.17}$$

We call $a_-$ the "annihilation operator" since there exists a state $\psi_0(x)$ such that $a_-\,\psi_0 = 0$, its Hermitian conjugate $a_+ = a_-^\dagger$ is called the "creation" operator. The product that appears in the Hamiltonian is the "number operator"[3]. Consider the bra-ket notation associated with these wave functions – we have $\psi_n(x) = \langle x|\psi_n\rangle$, and we know that, as an operator $a_-\,|\psi_0\rangle = 0$. We can write the effect of the creation and annihilation operators as:

$$a_+\,|\psi_n\rangle = \sqrt{n+1}\,|\psi_{n+1}\rangle \qquad a_-\,|\psi_n\rangle = \sqrt{n}\,|\psi_{n-1}\rangle \tag{15.18}$$

so that the number operator $N \equiv a_+\,a_-$, acting on $|\psi_n\rangle$ gives:

$$a_+\,a_-\,|\psi_n\rangle = a_+\,\sqrt{n}\,|\psi_{n-1}\rangle = n\,|\psi_n\rangle\,. \tag{15.19}$$

The integer label $n$, of course, is directly related to the energy of the state – the Hamiltonian operator acting on $|\psi_n\rangle$ is

$$H\,|\psi_n\rangle = \hbar\,\omega\left(n + \frac{1}{2}\right)|\psi_n\rangle\,, \tag{15.20}$$

and we sometimes use the label $n$ by itself inside the ket, as in $|0\rangle$, $|1\rangle$, $|2\rangle$, etc.

It is interesting to note that the states $|n\rangle$ are eigenkets of both $N$ and $H$ – as we can see from the above. This was achieved by construction, we found it easier to describe the factored form, and hence, the eigenkets of $a_+\,a_-$ than the Hamiltonian's eigenstates. But if we are to exploit this simplification in other areas, we should ask: How do we know that two operators share a common set of eigenkets?

The answer: When they *commute*. That is to say, if we have two operators $A$ and $B$, if

$$[A, B] = A\,B - B\,A = 0, \tag{15.21}$$

[3]Note that it is common to define $a \equiv a_-$ and then $a^\dagger$ is pretty obvious.

then the operators are "simultaneously diagonalizable", meaning in particular, that we can find a basis in which both operators are diagonalized[4]. This is clearly true for $H$ and $N$:

$$[H, N] = H\,N - N\,H = \hbar\,\omega\left(N + \frac{1}{2}\right)\,N - N\,\hbar\,\omega\left(N + \frac{1}{2}\right) = 0, \quad (15.22)$$

since $[N, N] = 0$ automatically.

### 15.3.1 States with Zero "Uncertainty"

We know how to compute expectation values, and the variance of operators, and we now understand that we are to associate Hermitian operators (with their real expectation values) with "measurement", so that the expectation value of an operator is supposed to correspond to measuring over and over on identical systems and averaging the results. We have seen that there are states, associated with any Hermitian operator, that return *precisely* a single value, with no variance whatsoever (called "determinate" states). These are the eigenstates of the operator itself, as we established when we found the stationary states for the infinite square well and harmonic oscillator – if you are in state $|0\rangle$, then you simply *have* energy $E_0 = \frac{1}{2}\,\hbar\,\omega$. The variance of the operator $H$ is:

$$\sigma^2 = \langle 0|\,H^2\,|0\rangle - (\langle 0|\,H\,|0\rangle)^2 = \left(\frac{1}{2}\,\hbar\,\omega\right)^2\,\langle 0|0\rangle - \left(\frac{1}{2}\,\hbar\,\omega\right)^2\,\langle 0|0\rangle\,. \quad (15.23)$$

The same argument holds for any operator with its eigenkets. From the previous section, we know that if two operators do not commute, then they do not share the same eigenkets, and hence determinant states of one operator *cannot be* determinant states of the other. This observation leads to the "uncertainty principle" – most famously applied to the operators $x$ and $p$ which have $[x, p] = i\,\hbar \neq 0$.

## 15.4 Statistical Interpretation

Our starting point was a statistical interpretation for the wavefunction $\Psi(x, t)$, whose dynamics is governed by the Schrödinger equation (in po-

[4] Notice what we are *not* saying is that an arbitrarily chosen eigenvector of $A$ is also an eigenvector of $B$ if $[A, B] = 0$ – that is not true. In general, it requires some work, given all eigenvectors of $A$ and $B$, to find a set that is common to both.

sition space). We have now seen that the spatial form is "just" a basis for the abstract vector $|\Psi\rangle$, namely $\Psi(x,t) = \langle x|\Psi\rangle$. We think of $|\Psi(x,t)|^2\,dx$ as the probability of finding a particle in the range $dx$, and we can write this as $|\langle x|\Psi\rangle|^2\,dx$. But that would seem to indicate that we could write $|\langle p|\Psi\rangle|^2\,dp$, and interpret this as the probability of finding a particle in a momentum range $dp$. Of course, we can – any operator $Q$ with continuous eigenfunctions $|q\rangle$ has $|\langle q|\Psi\rangle|^2\,dq$ as the probability of finding a particle with property $q$ (a measured value of $Q$-ness of the system) in a range $dq$ about the value $q$.

That's fine for continuous eigenkets, but what about the hallmark of quantum mechanics, discrete spectra? For example, the harmonic oscillator Hamiltonian operator has a discrete spectrum, yet the basis functions associated with the energy eigenstates are complete. Instead of having a projection that is continuous (like $\langle x|\Psi\rangle$), an arbitrary state can be made up out of an infinite *sum*:

$$|\Psi\rangle = \sum_j a_j\ |j\rangle\,, \tag{15.24}$$

and now we see that the projection $\langle j|\Psi\rangle$ gives us the coefficient $a_j$. So what do we make of a "measurement"? We don't have a $dE$, for example, an energy interval, since *the system must have one of the discrete energies.* That's a new element here, and part of the statistical interpretation for operators (measuring devices) having discrete spectra (quantized value). A measurement of energy for the harmonic oscillator will return a value $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$, for some integer $n$. We can still find the probability that we get a particular $E_n$, that is given by $|\langle j|\Psi\rangle|^2 = |a_j|^2$.

The above, while we are using the harmonic oscillator Hamiltonian and its discrete spectrum as an example, holds for any operator with a discrete spectrum. If we write the state $|\Psi\rangle$ in terms of the eigenkets of the operator, then $|\langle j|\Psi\rangle|^2$ will be the probability we get the $j^{th}$ eigenvalue. This is, again, the story we tell ourselves, a way of explaining experimental results, and a fundamental interpretive input into quantum mechanics. It is mathematically sensible, of course, the expectation value associated with, for example, energy reads, for $|\Psi\rangle = \sum_{j=1}^{\infty}\alpha_j\ |j\rangle$ (where $|j\rangle$ are the eigenkets of the Hamiltonian) :

$$\langle H\rangle = \langle\Psi|\ H\ |\Psi\rangle = \sum_j |a_j|^2\,E_j \tag{15.25}$$

assuming we have normalized the wave function. Our discrete probability interpretation is: We measure a value $E_j$ with probability $|a_j|^2$.

In general, the expectation value for an operator $Q$ (with eigenkets $|j\rangle$ having eigenvalue $q_j$) is

$$\langle Q \rangle = \langle \Psi | \, Q \, | \Psi \rangle = \langle \Psi | \sum_j a_j \, q_j \; | j \rangle = \sum_j |a_j|^2 \, q_j, \tag{15.26}$$

i.e. the probability of getting each eigenvalue weighted by the eigenvalue, just what we normally mean by an “average value”.

**Homework**

Reading: Griffiths, pp. 96–105.

**Problem 15.1**

Some problems (meaning, here, potentials) are easier to solve using the momentum form of Schrödinger's equation (15.7). Consider a constant force potential: $V(x) = -F\,x$.

**a.** Write Schrödinger's equation appropriate for $\Psi(p,t)$ with the potential in place (do not separate in $p$ and $t$).

**b.** Take the ansatz $\Psi(p,t) = P(p - F\,t)\,Q(p)$ for arbitrary $P(p - F\,t)$ and show that Schrödinger's equation simplifies to

$$\frac{dQ(p)}{dp} = -\frac{i\,p^2}{2\,m\,\hbar\,F}\,Q(p). \tag{15.27}$$

Solve this equation for $Q(p)$.

**c.** Using your full solution, $\Psi(p,t) = P(p - F\,t)\,Q(p)$ (input your $Q(p)$ from above), what is the probability density associated with momentum measurement: $\rho(p,t) = \Psi^*(p,t)\,\Psi(p,t)$? What does this tell you about $\int_{-\infty}^{\infty} |P(p - F\,t)|^2\,dp$?

**d.** Assuming we start in an initial state that has $\langle p \rangle = 0$, show that, using your time-dependent solution $\Psi(p,t)$, you get:

$$\langle p \rangle = F\,t, \tag{15.28}$$

consistent with a particle moving with constant force. Verify that Ehrenfest's theorem gives the same result.

**Problem 15.2**

We are familiar with the operators $x$, $p$ and $H$ (formed from the other two). Here we explore a new operator: $P$, the "parity" operator. It is defined by its action on a function (in Hilbert space):

$$P\, f(x) = f(-x). \tag{15.29}$$

**a.** Find the eigenvalues and associated eigenfunctions of $P$ – you want $f(x)$ such that $P\, f(x) = \alpha\, f(x)$ for $\alpha \in \mathbb{C}$. Hint: Try applying the parity operator to the eigenvalue equation.

**b.** Show that $P$ is a Hermitian operator: That is, show that

$$\int_{-\infty}^{\infty} f(x)^*\, P\, g(x)\, dx = \int_{-\infty}^{\infty} (P\, f(x))^*\; g(x)\, dx. \tag{15.30}$$

**c.** Show that two eigenfunctions of $P$, with different eigenvalue, are orthogonal: For $f(x)$ and $g(x)$ eigenfunctions of $P$ having different eigenvalues, you need to establish that:

$$\int_{-\infty}^{\infty} f(x)^*\, g(x)\, dx = 0. \tag{15.31}$$

**Problem 15.3**

Find the Hermitian conjugate of the operator

$$a_+ = \frac{1}{\sqrt{2\, m\, \hbar\, \omega}} \left( -\hbar\, \frac{d}{dx} + m\, \omega\, x \right), \tag{15.32}$$

by explicit construction:

$$\int_{-\infty}^{\infty} f(x)^*\, a_+\, g(x)\, dx = \int_{-\infty}^{\infty} \big( \underbrace{a_+^\dagger}_{?}\; f(x) \big)^*\, g(x)\, dx. \tag{15.33}$$