Linear Algebra in Hilbert Space

Lecture 14

Physics 342
Quantum Mechanics I

Wednesday, February 27th, 2008

We have seen the importance of the plane wave solutions to the potential-free Schrödinger equation. While not physically interpretable by themselves, they can be used to build up arbitrary solutions in the presence of simple potentials.

All of our work so far has been associated with solving the operator eigenvalue equation:

$$\hat{H}\psi(x) = E\psi(x) \tag{14.1}$$

the time-independent Schrödinger equation. But we have seen a number of operators, and their eigenvalues and eigenfunctions are also of interest – the idea is that any operator that commutes with $\hat{H}$ shares its spectrum – so it might be computationally simpler to develop the spectrum of a different operator.

We need some machinery to make this clear. While it is simple to show that for matrices $\mathbb{A}$ and $\mathbb{B}$, $[\mathbb{A}, \mathbb{B}] = 0$ implies a shared set of eigenvalues, what we mean by $[\hat{Q}, \hat{H}] = 0$ is less obvious.

14.1 Eigenvectors of x

We have been thinking of x as an operator, it "multiplies by x" in expressions like:

$$\int_{-\infty}^{\infty} \Psi(x,t)^* \, x \, \Psi(x,t) \, dx. \tag{14.2}$$

Can we find the eigenvalues and eigenvectors of x? What would this *mean*? Well, the eigenvector is some function which, when acted on by x returns a number times the function. Call the "number" $\bar{x}$, and the function $f_{\bar{x}}(x)$, then we want:

$$x\, f_{\bar{x}}(x) = \bar{x}\, f_{\bar{x}}(x). \tag{14.3}$$

In this expression, the x on the left is an *operator*, while the x appearing as the argument of $f_{\bar{x}}(x)$ is the argument of the function. Now the usual function we would associate with the above is $f_{\bar{x}}(x) = \delta(x - \bar{x})$. That certainly has the property that

$$x\, \delta(x - \bar{x}) = \bar{x}\, \delta(x - \bar{x}), \tag{14.4}$$

which is what we want. The "eigenvalue" $\bar{x}$ here is continuous, which is familiar from, for example, the "free particle" solutions to Schrödinger's equation.

Thinking back to the dot product we have been using for functions, we have, for two "different" eigenfunctions, $\mathbf{f}_{\bar{x}} \equiv f_{\bar{x}}(x)$ and $\mathbf{f}_{\hat{x}} \equiv f_{\hat{x}}(x)$ (with eigenvalues $\bar{x}$ and $\hat{x}$ respectively):

$$\mathbf{f}_{\bar{x}} \cdot \mathbf{f}_{\hat{x}} = \int_{-\infty}^{\infty} \delta(x - \bar{x})\, \delta(x - \hat{x})\, dx = \delta(\hat{x} - \bar{x}) = \delta(\bar{x} - \hat{x}) \tag{14.5}$$

since the delta function is symmetric. This is the analogue of our discrete cosine basis, for example, where we had $\mathbf{e}_m \cdot \mathbf{e}_n = \delta_{mn}$. And, just as we could decompose generic functions in the infinite (but discrete) basis set $\{\mathbf{e}_i\}_{i=1}^{\infty}$ by taking the weighted sum:

$$g(x) = \sum_{i=1}^{\infty} (g(x) \cdot \mathbf{e}_i)\, \mathbf{e}_i, \tag{14.6}$$

we can decompose a function $g(x)$ in the eigenvectors of the operator x:

$$g(x) = \int_{-\infty}^{\infty} \phi(\bar{x})\, f_{\bar{x}}(x)\, d\bar{x}, \tag{14.7}$$

to find the "coefficients" $\phi(\bar{x})$ in terms of this basis, we take the "projection of $g(x)$ onto the basis vector $\mathbf{f}_{\bar{x}}$":

$$g(x) \cdot \mathbf{f}_{\bar{x}} = \int_{-\infty}^{\infty} g(x)\, \delta(x - \bar{x})\, dx = g(\bar{x}), \tag{14.8}$$

so the values of $g(\bar{x})$ *are* the coefficients of $g(x)$ in the basis $\mathbf{f}_{\bar{x}}$. That is no surprise, we are specifying a function of x, meaning we are already in the basis associated with x.

The identity, analagous to the above (14.6) is

$$g(x) = \int_{-\infty}^{\infty} (g(x) \cdot \mathbf{f}_{\bar{x}})\, \mathbf{f}_{\bar{x}}\, d\bar{x}. \tag{14.9}$$

The eigenvectors of x clearly form a (trivial) complete basis for functions $f(x)$, and we see that the notation $f(x)$ itself is indicative of a projection onto this basis set. We might wonder, therefore, if a function $f(x)$ has a more abstract form which would facilitate representation in other bases (i.e. the eigenvectors of other operators).

14.2 Bra-Ket Notation

Dirac used a notation that freed him from committing to particular representations of "vectors", functions of x are the x-operator-eigenbasis representation of a vector. Just as we typically represent finite vectors in terms of their components *with respect to* a particular basis, and in the abstract as $\mathbf{a}$:

$$\begin{aligned} \mathbf{a} &= a_1\,\mathbf{e}_1 + a_2\,\mathbf{e}_2 + \ldots a_n\,\mathbf{e}_n \\ &\doteq \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \end{aligned} \tag{14.10}$$

he suggested using the abstract form $|a\rangle$ (called "ket a") to represent a vector in a space (be it function space or any other). In this language, the eigenvectors of x are denoted $|\bar{x}\rangle$ and we would write the eigenvector equation as

$$x\,|\bar{x}\rangle = \bar{x}\,|\bar{x}\rangle\,. \tag{14.11}$$

This makes the situation clear: $|\bar{x}\rangle$ is the eigenvector, x is the operator acting on it, and $\bar{x}$ is the eigenvalue.

In addition to $|\bar{x}\rangle$, he introduced the "bra", $\langle\bar{x}|$ which is the "Hermitian conjugate" of $|\bar{x}\rangle$ – in the language of finite vector spaces, we would say:

$$\begin{aligned} |a\rangle &\doteq \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \\ \langle a| &\doteq \begin{pmatrix} a_1^* & a_2^* & \ldots & a_n^* \end{pmatrix}. \end{aligned} \tag{14.12}$$

The representation for functions is slightly different – we typically form $\langle a|$ in preparation for a dot-product – defined to be $\langle a|b\rangle$, a natural expression in terms of the above column and row vectors. Without worrying, yet, about how the inner product is *defined*, take the object $\langle a|b\rangle$ to be an inner product, meaning that it satisfies the usual inner product relations ($\langle a|b\rangle = \langle b|a\rangle^*$, $\langle a|a\rangle$ is real, etc.).

Now consider the sentiment expressed in (14.8), we have a vector $|g\rangle$ in a function space, and we have the eigenvectors of the operator x, so we would write:

$$g(\bar{x}) = \langle \bar{x}|g\rangle \,, \tag{14.13}$$

i.e. the projection of the vector $|g\rangle$ onto the basis formed by $|\bar{x}\rangle$. We have used the $\langle \bar{x}|$ form to construct the inner product. Consider, then, the x-coordinate representation of the $|x\rangle$ ket *itself*:

$$f_{\bar{x}}(x) \equiv \langle x|\bar{x}\rangle = \delta(x-\bar{x}). \tag{14.14}$$

To be less oblique about all of this, consider writing (14.9) in bra-ket notation for the $|\bar{x}\rangle$ basis:

$$\begin{aligned} |g\rangle &= \int_{-\infty}^{\infty} \underbrace{|\bar{x}\rangle}_{\text{basis}} \quad \underbrace{\langle \bar{x}|g\rangle}_{\text{coefficients}} \quad d\bar{x} \\ &= \int_{-\infty}^{\infty} |\bar{x}\rangle \; g(\bar{x})\, d\bar{x} \end{aligned} \tag{14.15}$$

and this suggets that the unity operator is precisely:

$$1 = \int_{-\infty}^{\infty} |\bar{x}\rangle \, \langle \bar{x}| \; d\bar{x}. \tag{14.16}$$

We can now establish the usual function norm (or "L_2" norm) of two complex functions $f(x)$ and $g(x)$ – consider their vector form $|f\rangle$ and $|g\rangle$, then

$$\langle f|g\rangle = \int_{-\infty}^{\infty} \langle f|\bar{x}\rangle \, \langle \bar{x}|g\rangle \; d\bar{x} = \int_{-\infty}^{\infty} f(\bar{x})^* \, g(\bar{x})\, d\bar{x}, \tag{14.17}$$

precisely the sort of object we have been dealing with. In this notation, then, our expectation values look like:

$$\begin{aligned} \langle\psi|\, x \,|\psi\rangle &= \int_{-\infty}^{\infty} \psi(x)^* \, x \, \psi(x)\, dx \equiv \langle x\rangle \\ \langle\psi|\, p \,|\psi\rangle &= \int_{-\infty}^{\infty} \psi(x)^* \, p \, \psi(x)\, dx \equiv \langle p\rangle \end{aligned} \tag{14.18}$$

14.3 Other Bases

Of course, x is not the only operator on the block. We know the momentum operator, and we can work out its eigenvectors in position space – for the operator p, we have

$$p\, f_{\bar{p}}(x) = \bar{p}\, f_{\bar{p}}(x) \tag{14.19}$$

so that

$$\frac{\hbar}{i}\,\frac{df_{\bar{p}}(x)}{dx} = \bar{p}\, f_{\bar{p}}(x) \longrightarrow f_{\bar{p}}(x) = \alpha\, e^{\frac{i\,p\,x}{\hbar}}. \tag{14.20}$$

The momentum eigenkets $|\bar{p}\rangle$, written in the position basis are:

$$\langle \bar{x}|\bar{p}\rangle = \alpha\, e^{\frac{i\,\bar{p}\,\bar{x}}{\hbar}} \tag{14.21}$$

for some constant α. Incidentally, this is the complex conjugate of the position eigenvectors $|\bar{x}\rangle$ written in the momentum basis (since $\langle \bar{p}|\bar{x}\rangle = \langle \bar{x}|\bar{p}\rangle^*$). There is a notion of orthonormality here, and we can use this to set α. Consider:

$$\begin{aligned}\langle p|\bar{p}\rangle &= \int_{-\infty}^{\infty} \langle p|\bar{x}\rangle\; \langle \bar{x}|\bar{p}\rangle\; d\bar{x} \\ &= \int_{-\infty}^{\infty} \alpha^2\, e^{i\,\frac{\bar{x}\,(\bar{p}-p)}{\hbar}}\; d\bar{x} \\ &= \alpha^2\, 2\,\pi\,\hbar\,\delta(p-\bar{p})\end{aligned} \tag{14.22}$$

so set $\alpha = \frac{1}{\sqrt{2\,\pi\,\hbar}}$. This tells us the representation of the ket $|\bar{p}\rangle$ in the momentum basis (just as $\langle x|\bar{x}\rangle = \delta(x-\bar{x})$ was the representation of the ket $|\bar{x}\rangle$ in the position basis):

$$f_{\bar{p}}(p) = \delta(p-\bar{p}). \tag{14.23}$$

We have the same notion of completeness as we had for $|\bar{x}\rangle$ – if we represent a function in the momentum basis, $g(p) = \langle p|g\rangle$, then

$$|g\rangle = \int_{-\infty}^{\infty} \underbrace{|\bar{p}\rangle}_{\text{basis}}\quad \underbrace{\langle \bar{p}|g\rangle}_{\text{coefficients}}\quad d\bar{p} \tag{14.24}$$

so we can again write the unity operator as:

$$1 = \int_{-\infty}^{\infty} |\bar{p}\rangle\, \langle \bar{p}|\; d\bar{p}. \tag{14.25}$$

But what is the relation between functions written in the position and momentum basis? We are imagining $|f\rangle$, a vector that is in the function space, and we have just established that we can project this vector onto the basis $|\bar{x}\rangle$ or $|\bar{p}\rangle$, there "must" be some deep connection between functions represented in these two bases.

Suppose we want to take a function of position $f(x)$ and write it in the momentum basis:

$$g(\bar{p}) = \langle \bar{p}|g\rangle = \int_{-\infty}^{\infty} \langle \bar{p}|\bar{x}\rangle \, \langle \bar{x}|g\rangle \, d\bar{x} \quad = \frac{1}{\sqrt{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} e^{-\frac{i\,\bar{p}\,\bar{x}}{\hbar}} \, g(\bar{x})\, d\bar{x}, \tag{14.26}$$

evidently, the momentum basis representation of $|g\rangle$ is just the Fourier transform of its position representation (modulo a factor of $\hbar$).

Similarly, we can write the position representation in terms of the momentum one:

$$g(x) = \langle x|g\rangle = \int_{-\infty}^{\infty} \langle x|\bar{p}\rangle \, \langle \bar{p}|g\rangle \, d\bar{p} = \frac{1}{\sqrt{2\,\pi\,\hbar}} \int_{-\infty}^{\infty} e^{\frac{i\,\bar{p}\,x}{\hbar}} \, g(\bar{p})\, d\bar{p}, \tag{14.27}$$

confirming that the position representation is the Fourier transform of the momentum representation, as expected.

Which of these is the "real" wavefunction? It's great that we can write $|\psi\rangle$, for example, and then talk about $\langle p|\psi\rangle$ or $\langle x|\psi\rangle$, but what is $|\psi\rangle$? This is the same as asking what a vector $\mathbf{a}$ is – we can choose a basis and represent the decomposition of $\mathbf{a}$ in terms of that basis, but without *some* basis, it is difficult to say much beyond "$\mathbf{a}$ is an element of a vector space." In our case, we have been primarily interested in the Schrödinger equation written in position space, so the familiar object is $\Psi(x,t)$, a function of position. Then we have been dealing implicitly with $\Psi(x,t) = \langle x|\Psi(t)\rangle$ for a ket $|\Psi(t)\rangle$.

14.4 Hilbert Space

We have been referring to "a function space" or even "the function space" as if it has been defined. What we mean is Hilbert space.

Our wavefunctions satisfy the property

$$\int_{-\infty}^{\infty} \Psi(x,t)^* \, \Psi(x,t)\, dx = \langle \Psi(t)|\Psi(t)\rangle = 1 \tag{14.28}$$

so that they are "square integrable" for all times t (guaranteed by Schrödinger's equation). The set of all such functions forms a vector space called "Hilbert Space". Neither the eigenvectors of position nor momentum are actually *in* the Hilbert space, but they still form a basis for it – that's life in infinite dimensional vector spaces.

More generally, a Hilbert space on an interval $[a, b]$ is the set of all complex functions $f(x)$ defined for $x \in [a, b]$ with the property that:

$$\int_a^b |f(x)|^2 \, dx = A \tag{14.29}$$

for finite A.

The eigenkets of the x and p operators are clearly convenient, but there are other natural bases that are better behaved: For a discrete basis (akin to the cosine or sine series, these exist in Hilbert space for some finite domain) we have an infinite set of basis kets $|e_i\rangle$ with $\langle e_i|e_j\rangle = \delta_{ij}$, and we can explicitly form:

$$|f\rangle = \sum_{i=1}^{\infty} a_i \, |e_i\rangle \,, \tag{14.30}$$

then our notation tells us that

$$\langle e_i|f\rangle = \int_{-\infty}^{\infty} \langle e_i|x\rangle \, \langle x|f\rangle \, dx = \int_{-\infty}^{\infty} e_i^*(x) \, f(x) \, dx = a_i. \tag{14.31}$$

Homework

Reading: Griffiths, pp. 93–96.

Problem 14.1

This problem is meant to suggest an association between the ill-defined $\int_{-\infty}^{\infty} e^{i\,k\,(x-a)}\,dk$ and the Dirac delta function: $\delta(x-a)$.

a. Define

$$f_n(x) \equiv \frac{1}{2\,\pi} \int_{-n}^{n} e^{i\,k\,(x-a)}\,dk, \tag{14.32}$$

show that $\int_{-\infty}^{\infty} f_n(x)\,dx = 1$ for all n (you may find the definite integral: $\int_0^{\infty} \frac{\sin(y)}{y}\,dy = \frac{1}{2}\,\pi$ useful).

b. Show that the value of $f_n(a) \to \infty$ as $n \to \infty$. It should also be clear that values other than $x = a$ are small in comparison to ∞.

Problem 14.2

Find the eigenfunctions of the lowering operator:

$$a_- \equiv \frac{1}{\sqrt{2\,m\,\hbar\,\omega}} \left(\frac{d}{dx} + m\,\omega\,x\right), \tag{14.33}$$

that is, find functions $f_\alpha(x)$ such that $a_-\,f_\alpha(x) = \alpha\,f_\alpha(x)$.

Problem 14.3

Griffiths Problem 3.2. Here we are looking at what does and does not live in Hilbert space.