VII. HILBERT SPACE

Last time we found the range of allowed energies for a particle in a box, and the allowed wave functions. The allowed energies are actually the eigenvalues of a linear operator, with the functions being eigenvectors. But in what space? In function space. Mathematically, the appropriate construction is a Hilbert space.

A. Definition of a Hilbert space

A Hilbert space is:

1. An infinite-dimensional vector space.
2. has a norm.
3. has an inner product.

Wait - what are the vectors in the problem? These are the wave functions:

$$\psi_n(x) = A_n \sin(k_n x) \tag{133}$$

You can think of them as an infinite dimensional vector, with the dimension index being the location in space, and the entres being the function itself:

$$\{\psi_n(x)\}_{x=0}^{L} \tag{134}$$

What would serve as a norm? Easy to guess:

$$(\psi_n, \psi_n) = \int dx \psi(x)^* \psi(x) \tag{135}$$

We should work with normalized vectors, so:

$$(\psi_n, \psi_n) = \int dx A_n^2 \sin^2(k_n x) = \frac{L}{2} A_n^2 \tag{136}$$

So choosing:

$$A_n = \sqrt{2/L} \tag{137}$$

does the trick.

How about an inner product (i.e., the usual dot product)? You guessed it again:

$$(\psi_n, \psi_m) = \int dx \psi_n(x)^* \psi_m(x) \tag{138}$$

By the way, in this case, what is the answer? Let's do it:

$$(\psi_n, \psi_m) = \int_0^L dx \frac{2}{L} \sin(n\pi x/L) \sin(m\pi x/L) = \int_0^L dx \frac{-2}{4L} (e^{i(n+m)\pi/L} + e^{-i(n+m)\pi/L} - e^{i(n-m)\pi/L} + e^{-i(n-m)\pi/L}) = \delta_{nm} \tag{139}$$

So this set of vectors is orthonormal.

B. Dirac Notation: Bra's and ket's

Now, instead of using the usual notation - something like $\vec{\psi}_n$ for these Hilbert space vectors, Dirac suggested to call them Bra and Ket, as a short for Bracket. You can see the ubiquity of brackets inthe discussion above. The ket is supposed to signify the latter part of the bracket:

$$, \psi_n) \to |n\rangle \tag{140}$$

and the bra supposed to be the beginning part:

$$\psi^* \sim (\psi_n, \rightarrow \langle n| \tag{141}$$

The kets should remind you of column vectors, and the bras as their hermitian conjugate: complex conjugated row vectors. So in particular:

$$|n\rangle = \langle n|^\dagger \tag{142}$$

where the dagger indicates hermitian conjugate.

And now everything follows. For instance, the orthonormality condition reads:

$$\langle n|\, m\rangle = \delta_{nm} \tag{143}$$

Furthermore, if you'd like to describe a function as a superposition of the eigenstates, ψ_n, which here coincides with a Fourier series, we write:

$$|v\rangle = \sum_n v_n \,|n\rangle \tag{144}$$

As an example, let's try to make the normalization condition on this representation:

$$\begin{aligned}\langle v|\, v\rangle = \left(\sum_n v_n\,|n\rangle\right)^\dagger \left(\sum_m v_m\,|m\rangle\right) = \left(\sum_n v_n^*\,\langle n|\right)\left(\sum_m v_m\,|m\rangle\right) \\ = \sum_{nm} v_n^* v_m\,\langle n|\, m\rangle = \sum_{nm} v_n^* v_m \delta_{nm} = \sum_n v_n^* v_n\end{aligned} \tag{145}$$

So normalization would require:

$$\sum_n v_n^* v_n = 1 \tag{146}$$

No surprise. So the ket $|v\rangle$ really can be thought of as a column vector, in the basis specified by $|n\rangle$.

C. Fourier series and completeness

as it turns out, the set of eigenstates that solve the TISE form a complete set. They can approximate any function.

Suppose we would like to write a function as a linear combination of these eigenstates - say a step function, how do we do this? Given a function $|f\rangle = f(x)$, we can write the following:

$$|f\rangle = \sum_n |n\rangle\, f_n \tag{147}$$

To find f_n we simply multiply from the right with $\langle m|$ and obtain:

$$\langle m\,|f\rangle = \sum_n \langle m\,|n\rangle\, f_n = \sum_n \delta_{mn} f_n = f_m \tag{148}$$

Now we can calculate the complete set of amplitude of the various components f_n. They are simply the 'Fourier components' calculated by integrating the integral of the eigenfunction with the function you wish to calculate.

How well is does this series do in approximating the function $f(x)$? How fast does the sum over all basis wave functions converge? To find out, we first define

$$f^{(N)} = \sum_{n=1}^{N} |n\rangle\, f_n \tag{149}$$

as a artial aproximation of f.

How good is this approximation? Is the distance

$$|f^{(N)}(x) - f(x)| \tag{150}$$

bounded in any way? No. It *can not* be proven to be smaller than some ϵ_N which obeys $\epsilon_N \to 0$ with N increasing. This implies that this approximation does not *uniformly converge* to $f(x)$.

What we can say, however, is that the decomposition is a good approximation with respect to the Hilbert space norm. The norm of the deviation is small:

$$\int |f^{(N)}(x) - f(x)|^2 < \epsilon_N \tag{151}$$

And certainly $\epsilon_N \to 0$ as $N \to \infty$.

D. Resulotion of the identity

Now that we got that out of the way, let me rewrite the decomposition in a rather disturbing way:

$$|f\rangle = \sum_n |n\rangle f_n = \sum_n |n\rangle \langle n| f\rangle = (\sum_n |n\rangle \langle n|) |f\rangle \tag{152}$$

This is funny. We now collected all the n-dependent pieces into a single operator:

$$I = \sum_n |n\rangle \langle n| \tag{153}$$

And because $|f\rangle$ survives unscathed, it means that I is the *identity matrix*. Eq. (153) is called the *resolution of the identity*. It is also a testament to the completeness of the $|n\rangle$ basis. If the basis were not complete, the operator I would have a kernel.

E. Operators

We discussed vectors and rewrote them in terms of bras and kets. The remaining element of the construction of a vectors space is the operators. So far we so several exapmples of operators. Can you name a few?

$$\hat{x},\, \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x},\, \hat{x}^2, \ldots \tag{154}$$

The hamiltonian itself is also an operator. Also so far, we calculated their expectation values:

$$\langle \hat{x} \rangle = \int dx \psi^* x \psi \tag{155}$$

Now we see that in our new notation this is:

$$\langle \hat{x} \rangle = (\psi, \hat{x}\psi) = \langle \psi | \hat{x}\psi \rangle = \langle \psi | \hat{x} |\psi\rangle \tag{156}$$

More than anything, though, the operators are matrices. For instance, when we operate with the operator $\hat{x}$ on $|n\rangle$ we would get:

$$\hat{x} |n\rangle = x_{mn} |m\rangle \tag{157}$$

This could be read easily from the functional representation of this equation:

$$\hat{x} |n\rangle = x\sqrt{2/L} \sin(n\pi x/L) \tag{158}$$

The new function can be expanded in terms of the complete set that the solutions of he square well potential present. How do we find the expansion coefficients? simply by taking the contraction:

$$x_{mn} = \langle m | \hat{x} |n\rangle \tag{159}$$

The operator $\hat{x}$ is a prime example of an Hermitian matrix. To understand hermiticity in the Dirac notation, we need to go throuh a few stages. First, let's ask, what is x_{nm} in terms of x_{mn}:

$$x_{nm} = \int_0^L dx \psi_n^* (x\psi_m) \tag{160}$$

To change the order, we first must take a complex conjugate:

$$x^*_{nm} = \int_0^L dx (x\psi_m)^* \psi_n = \int_0^L dx (\psi_m)^* x \psi_n = x_{mn} \tag{161}$$

So if we write is as a matrix, the transpose is the complex conjugate of the original:

$$\hat{x} = (\hat{x}^T)^* = \hat{x}^\dagger \tag{162}$$

by definition this is the adjoint.

Actually th momentum is another prime example of an Hermitian operator:

$$p^*_{nm} = \int_0^L dx (\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_m)^* \psi_n = \int_0^L dx \left(-\frac{\hbar}{i}\right) \frac{\partial \psi^*_m}{\partial x} \psi_n \tag{163}$$

by integration by parts we get:

$$= \int_0^L dx \psi_m \left(\frac{\hbar}{i}\right) \frac{\partial \psi_n}{\partial x} = p_{mn} \tag{164}$$

F. statistical interpretation

Hermitian matrices have special properties. They are exactly diagonalizable. Furhtermore, all their eigenvalues are real numbers. We can therefore write them as follows:

$$\hat{A} = \sum_n \lambda_n |\lambda_n\rangle \langle \lambda_n| \tag{165}$$

assuming that the kets are completely normalized.

Furthermore, a wave function can always be broken down in terms of these:

$$|\psi\rangle = \sum_n a_n |\lambda_n\rangle \tag{166}$$

what are the coefficients a_n?

$$a_n = \langle \lambda_n | \psi \rangle. \tag{167}$$

Now, we talked about operators as matrices. We showed that the common ones are hermitian. Actually, all physical observavles should be Hermitian operators. Why? Because they must have real expectation values.

One more math question. given an observable $\hat{A}$, what is its expectation value in terms of the a_n's? That's quite straightforward:

$$\langle \psi | \hat{A} | \psi \rangle = \ldots = \sum_n \lambda_n |a_n|^2 \tag{168}$$

What is then the interpretation of the $|a_n|^2$? A probability distribution.

But then, what is the meaning of the eigenvalues? These are the only allowed values that the quantum theory permits. This should not surprise us too much. For instance:

$$\hat{H} = \sum_n E_n |n\rangle \langle n| \tag{169}$$

dictates the energy spectrum of the particle in a box.

what about $\hat{p}^2$ for the particle in a box? clearly this is a diagonal operator, with eigenvalues:

$$k_n^2 = \left(\frac{\pi}{L} n\right)^2 \tag{170}$$

G. Commutators

Quick question: is $\hat{x}\hat{p}$ Hermitian? If they were matrices, would this combination be hermitian? Actually not. If we think of these as matrices (which they are!) we would have:

$$(\hat{x}\hat{p})^\dagger = \hat{p}^\dagger \hat{x}^\dagger = \hat{p}\hat{x} \tag{171}$$

Note the change in order! Acutally, what is the difference between the two? Think about them as operating on a non-existent function

$$(\hat{p}\hat{x} - \hat{x}\hat{p})\cdot = \frac{\hbar}{i}\frac{\partial}{\partial x}(x\cdot) - x\frac{\hbar}{i}\frac{\partial\cdot}{\partial x} \tag{172}$$

The derivative operates an extra time on x in the first term. This is the only thing which holds back this term from being zero:

$$= -i\hbar\cdot \tag{173}$$

This statement is of great importance, we call this difference teh *commutator*:

$$[p, x] = -i\hbar. \tag{174}$$