Physics 342 Lecture 6

Welcome to the course that is getting closer to quantum mechanics each lecture! Please turn in your first homework. The second homework is now assigned and due next friday.

At the end of the previous lecture, we had defined the Hilbert Space as a complex vector space consisting of those vectors of length 1. We can denote the Hilbert space as script H, $\mathcal{H}$, and so is

$$\mathcal{H} = \{ \vec{b} \in \mathbb{C}^N \mid \vec{b}^\dagger \vec{b} = 1 \}$$

For the Hilbert space of continuous functions, this is

$$\mathcal{H} = \{ g(x) \in \mathbb{C},\ x \in \mathbb{R} \mid \int dx\, g^*(x)\, g(x) = 1 \},$$

which means that a function $g(x)$ in the Hilbert space is L^2-normalized.

Linear operators act on states/vectors/functions in the Hilbert space, mapping them to other vectors. We had shown that a linear operator/matrix $\mathbb{M}$ maps an element $\vec{b}$ of the Hilbert space to another element of $\mathcal{H}$, say $\vec{c}$, if $\mathbb{M}$ is a unitary matrix; that is a matrix for which:

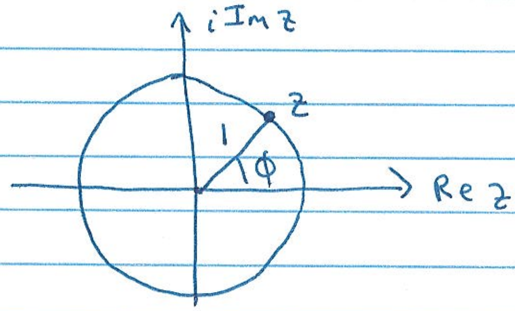
$$\mathbb{M}^\dagger \mathbb{M} = \mathbb{I},$$ where $\dagger$ means Hermitian conjugation (transposition and complex conjugation).

Because unitary matrices/operators map the Hilbert space to itself, they will have a central importance in what follows.

So, let's work to understand these unitary operators in detail. First, what does "unitary" mean? Well "unit" means "one", so somehow a unitary matrix represents "one", or so its name would suggest. To get a sense for this, let's just consider what a 1×1 unitary "matrix" would be. A 1×1 matrix is just a number, and as such is its own transpose. Let's call this number z, say, and so $z^T = z$. Then, the unitary constraint on z is just

$$z^\dagger z = z^* z = |z|^2 = 1.$$

A complex number with unit length is just some number on the unit circle:



z can therefore be written as:

$$z = e^{i\phi} = \cos\phi + i\sin\phi.$$

Thus, we can interpret "unitary" to mean of unit length or magnitude.

Can we use this insight from just regular complex numbers to understand general $N \times N$ unitary matrices? Let's take a hint from the exponential form of $z = e^{i\phi}$ and attempt to write a unitary matrix $\mathbb{M}$ as:

$$\mathbb{M} = e^{i\mathbb{T}}, \text{ for some } \underline{\text{other}} \text{ matrix } \mathbb{T}.$$

As always with the exponential, we really think of it through its Taylor expansion. That is, exponentiating a matrix T means:

$$e^{iT} = \mathbb{I} + iT - \frac{T^2}{2} - i\frac{T^3}{6} + \dots = \sum_{n=0}^{\infty} \frac{i^n}{n!} T^n.$$

In this way, every ~~element~~ term of the Taylor expansion is just found by matrix multiplication of T with itself a number of times. The first term in the Taylor expansion is now the identity matrix $\mathbb{I}$, the generalization of 1 to $N \times N$ matrices.

So, with this form of $\mathbb{M}$, let's see what the constraint on T is. Recall that, for $z = e^{i\phi}$, ϕ must be real for z to have unit magnitude. So, what is the generalization of a real number to matrices? It is not that every element of the matrix is real. Recall ~~matrix~~ individual matrix elements are basis-dependent and are not intrinsic properties of the matrix...

So, let's just Hermitian conjugate $\mathbb{M} = e^{iT}$ and see what we find. We find

$$\mathbb{M}^\dagger = \left(e^{iT}\right)^\dagger = \left(\mathbb{I} + iT - \frac{T^2}{2} - i\frac{T^3}{6} + \dots\right)^\dagger$$

$$= \sum_{n=0}^{\infty} \left(\frac{i^n}{n!} T^n\right)^\dagger = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} (T^\dagger)^n = e^{-iT^\dagger}.$$

Note that both complex conjugation and transposition can be applied term-by-term in the Taylor expansion. So, we multiply:

$$\mathbb{M}^\dagger \mathbb{M} = e^{-iT^\dagger} e^{iT} = e^{i(T - T^\dagger)} = \mathbb{I}.$$

Now, we've done something a bit tricky in the second equality: we just added the exponents of the two factors on the left. We'll see next week that this isn't in general allowed when we exponentiate matrices, but it works in this case just fine. So, we must have:

$$\mathbb{I} = e^{i(T-T^\dagger)} = \mathbb{I} + i(T-T^\dagger) - \frac{(T-T^\dagger)^2}{2} + \cdots$$

The only way that this equality can hold is if the matrix T is equal to its Hermitian conjugate:

$T = T^\dagger$. Such a matrix is called a "Hermitian matrix" and, apparently, is the generalization of a real number to matrices.

We said that the individual matrix elements of a matrix T, say, is not intrinsic to the matrix; only its eigenvalues are. So, what are the eigenvalues of a Hermitian matrix? The eigenvalue equation for the matrix T is:

$T\vec{v} = \lambda\vec{v}$, for an eigenvector $\vec{v}$.

Now, let's Hermitian conjugate both sides of this expression:

$$(T\vec{v})^\dagger = \vec{v}^\dagger T^\dagger = (\lambda\vec{v})^\dagger = \lambda^* \vec{v}^\dagger$$

However, if T is Hermitian, $T^\dagger = T$, so this is just

$\vec{v}^\dagger T = \lambda^* \vec{v}^\dagger$.

However, as we've discussed, if we multiply a complex vector on the left of the matrix, then we must complex conjugate and transpose. That is,

$\vec{v}^\dagger T = \lambda \vec{v}^\dagger$, but the Hermitivity of T then enforces that the eigenvalue λ is equal to its complex conjugate:

$\lambda = \lambda^*$. That is, the eigenvalues of a Hermitian operator/matrix are <u>real</u> numbers. <u>This</u> is the generalization of real numbers to matrices. A <u>real</u> (i.e., Hermitian) matrix has exclusively real eigenvalues. As the only intrinsic properties of a matrix are its eigenvalues, this defines a Hermitian matrix, given any basis in which it expressed.

So, summarizing what we have so far, unitary matrices $\mathbb{M}$ such that

$$\mathbb{M}^\dagger \mathbb{M} = \mathbb{I}$$

map vectors in the Hilbert space to other vectors in the Hilbert space. The unitary matrix $\mathbb{M}$ can be further written as:

$$\mathbb{M} = e^{iT},$$

for some Hermitian matrix T such that:

$$T = T^\dagger.$$

The eigenvalues of a Hermitian matrix are exclusively real, even if the matrix itself is complex (i.e., has complex elements in a given basis).

Before we keep going, let's see some simple examples of Hermitian matrices to gain some intuition. Let's consider the 2x2 matrix:

$T = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. This is indeed Hermitian: as it is real, complex conjugation does nothing. Further, it is a symmetric matrix (equal to its transpose) and so is Hermitian. The eigenvalues can be ~~imme~~ immediately read off to be $\lambda = \pm 1$.

Now, consider the matrix: $T = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

This is an imaginary matrix for which its transpose is negative of itself: $T^T = -T$. However, complex ~~conjg~~ conjugation transforms $i \to -i$ and so this matrix is indeed Hermitian:

$$T^\dagger = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^* = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = T.$$

Now, to calculate the eigenvalues of T, we will use a trick that works for 2x2 matrices. The determinant of a matrix is its product of eigenvalues:

$$\det T = \lambda_1 \lambda_2 = -1, \quad \text{because } \det T = 0 \cdot 0 - i(-i) = -1.$$

Also, the trace of a matrix, the sum of its diagonal elements, is the sum of eigenvalues:

$$\operatorname{tr} T = \lambda_1 + \lambda_2 = 0 + 0 = 0.$$

Thus, $\lambda_2 = -\lambda_1$ and $\lambda = \pm 1$, which are indeed real numbers.

Now, we've seen operators with exclusively real eigenvalues before. Our momentum operator, $\hat{p}$, had real eigenvalues:

$$\hat{p}\, h_p(x) = \left(-ic_1 \frac{\partial}{\partial x}\right) h_p(x) = p\, h_p(x), \text{ where } p \in \mathbb{R}.$$

We had also provided a pleasing physical interpretation of the momentum operator, $\hat{p}$, from which we gave ~~its~~ its name. The momentum operator acts on an eigenfunction

$$h_p(x) = e^{i\frac{px}{c_1}},$$

and returns the, um, momentum eigenvalue of the function. Momentum is something that we can measure in a lab, and just like our block on a ramp, the momentum of some object is independent of the coordinate system we set up. Momentum is intrinsic to an object in the natural world, and correspondingly the eigenvalues p are intrinsic to the momentum operator $\hat{p}$.

Now, all eigenvalues of $\hat{p}$ are real, which would suggest that $\hat{p}$ is a Hermitian operator. However, while $T^\dagger = T$ means that all eigenvalues are real, the converse isn't necessarily true. So, let's see if the momentum operator is Hermitian, but just explicitly evaluating matrix elements of $\hat{p}$. $\hat{p}$ is Hermitian if the matrix elements $(\hat{p})_{ij}$ and $(\hat{p})_{ji}$ are related as:

$$(\hat{p})_{ji} = (\hat{p})^*_{ij}.$$

Let's calculate these matrix elements:

$$(\hat{p})_{ji} = \int dx\, f_j^*(x)\, \hat{p}\, f_i(x) = \int dx\, f_j^*(x)\left(-ic_1 \frac{\partial}{\partial x}\right) f_i(x)$$

$$\overset{\text{IBP}}{=} -ic_1\left[\int dx \frac{\partial}{\partial x}\left(f_j^*(x)\, f_i(x)\right) - \int dx\, f_i(x)\frac{\partial}{\partial x} f_j^*(x)\right]$$

$$= \int dx\, f_i(x)\left(ic_1 \frac{\partial}{\partial x}\right) f_j^*(x) = (\hat{p})_{ij}^*$$

On the second line we use integration by parts to move the derivative from $f_i(x)$ onto $f_j^*(x)$. The total derivative term integrates to the value of the functions on the boundary of the domain of x:

$$\int_{x_{min}}^{x_{max}} dx \frac{\partial}{\partial x}\left(f_j^*(x)\, f_i(x)\right) = f_j^*(x_{max})\, f_i(x_{max}) - f_j^*(x_{min})\, f_i(x_{min}).$$

We will assume that this vanishes, and we'll see explicit examples of this later. With this assumption, we indeed find that:

$$(\hat{p})_{ji} = (\hat{p})_{ij}^*,$$

and so $\hat{p}^\dagger = \hat{p}$, and the momentum operator is Hermitian.

With all these pieces, we then have a profound interpretation which we will exploit next week. Unitary operators map the Hilbert space to itself, and unitary operators can be expressed as exponentiation of Hermitian operators. The only basis-independent information of an operator are its eigenvalues and a Hermitian operator has exclusively real eigenvalues. The outcomes of physical experiment must both be 1) real numbers and 2) independent of basis, So, as suggested by studying the momentum operator, the eigenvalues of a Hermitian operator on a Hilbert space correspond to the results of a physical measurement. We thus also refer to these Hermitian matrices as, simply, "observables."

We'll keep going down this road next week...