Phys 412-1 Quantum Mechanics

(Dated: 2022 Fall)

Abstract

This document contains the TA notes for the course Phys 412-1 Quantum Mechanics in the fall quarter of the academic year 2022-2023.

CONTENTS

I. DISCUSSION 1 (SEP 29)

What is an observable? It is an *abstract operator* which can be *represented* in a matrix in terms of some entries using a suitable *basis*. Suppose we have an observable A. The matrix representation of A is hermitian. We need to know what we are talking about when we say a matrix is hermitian.

Hermitian matrices have the three important properties:

- They have *real eigenvalues*.
- Their *eigenvectors* are *orthogonal* [1].
- Their eigenvector form a *complete basis*.

The last item is purely mathematical but it is physically useful.

Now suppose I want to write down the eigenvalue equation for my operator A:

$$A|n\rangle = a_n|n\rangle \tag{1}$$

I'll be very simplistic in my notation and just put the quantum number into my kets and bras. A more proper notation is for the eigenkets is $|A;n\rangle$; namely, you'd indicate the operator, as well. Now, here we know that $a_n \in \mathbb{R}$ for all n [2]. As for the eigenkets, we know that they are orthogonal. But let's not worry about the magnitudes, so suppose everything is normalized. Then, we have the orthonormality relation

$$\langle n|m\rangle = \delta_{nm} \tag{2}$$

Let's talk about the completeness now. But to do that, I'll introduce the *projection operator*, Λ_n. Suppose I write down an operator like $|n\rangle\langle m|$. What does this guy do for a living? It is clearly not a ket vector due to the bra on the right. It is a tensor, which can be represented by some matrix in a proper basis. Consider the operator $|n\rangle\langle n|$. What does

this do? If I give you a generic state ket, say $|\psi\rangle$ and tell you to act this operator on this state, you'd get

$$|n\rangle\langle n| = |n\rangle\langle n|\psi\rangle \tag{3}$$

The second factor on the right, i.e. $\langle n|\psi\rangle$, is certainly a scalar. We have a ket, $|n\rangle$, next to it, so the operator $|n\rangle\langle n|$ most certainly produces this ket, times some complex number. We call this number, the *probability amplitude* (or the *transition amplitude*). It measures *how much* $|n\rangle$ *is contained in* $|\psi\rangle$, for lack of a better explanation. This is no different than the usual projection of vector. Suppose I have this vector $\boldsymbol{v}$ and I want to project it onto an axis in the direction of some other vector $\boldsymbol{n}$. Then, we express this new, projected vector as $(\boldsymbol{v}\cdot\hat{\boldsymbol{n}})\hat{\boldsymbol{n}}$, where I normalized my direction vector. This object, $\langle n|\psi\rangle$ has 1:1 correspondence to the object $\hat{\boldsymbol{n}}\cdot\boldsymbol{v}$.

The moral of the story is, $|n\rangle\langle n|$ projects any state onto the state $|n\rangle$. We define our projection operator then as

$$\Lambda_n := |n\rangle\langle n| \tag{4}$$

Let's study some properties of this projection operator. What happens if I act $\Lambda_n\Lambda_m$ ($m \neq n$) on some general state $|\psi\rangle$? Without doing explicit mathematics, we immediately see that we get zero. The reason is, we project our initial state onto $|m\rangle$ first, but then we try to project this ket onto $|n\rangle$. We cannot do that since our eigenkets are orthogonal. Let's prove this mathematically:

$$\Lambda_n\Lambda_n|\psi\rangle = |n\rangle\langle n|m\rangle\langle m|\psi\rangle \tag{5}$$

This is equal to zero because $\langle n|m\rangle = 0$. Suppose now I act Λ_n on $|\psi\rangle$ twice. What do I get? I get $|n\rangle$ again. Once I'm in this state, I don't go anywhere. So we may write

$$\Lambda_n\Lambda_m = \Lambda_n\delta_{nm} \tag{6}$$

Now let's go back to the completeness. Suppose I have this vector $\boldsymbol{v}$ in $3D$. How do I get the components along the Cartesian axes? I take the dot product of the vector and tack in the unit vector in that direction. So I'm actually projecting my vector onto all these axes. I also know that the three-dimensional real space is spanned by $\{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$ *completely*. There is no vector left out. You can express any vector using these unit vectors. An identical

story takes place here. If I have a general state $|\psi\rangle$, then, in order to be able express it using the eigenkets of this operator A, I need to project it onto each and every one of these eigenkets:

$$|\psi\rangle = |1\rangle\langle 1|\psi\rangle + |2\rangle\langle 2|\psi\rangle + \cdots = \sum_n |n\rangle\langle n|\psi\rangle = \sum_n \Lambda_n |\psi\rangle \tag{7}$$

We have discovered something now. Notice that we have $|\psi\rangle$ on both sides, namely a *vector* equal to itself with some operator in front. This can mean only one thing:

$$\sum_n \Lambda_n = \mathbb{1} \tag{8}$$

This is called the *completeness* relation. Inserting a sum of eigenkets and bras between two operators, which we'll do every now and then, is called the *resolution of identity*.

* * *

I like my projection operators because that's how I (used to) compute my transitions (and hopefully we'll do it together in the third quarter). If I want to measure the probability of an event taking place between some initial and final states, I immediately write down the transition amplitude as

$$T_{f\leftarrow i} = \langle f|\Lambda|i\rangle \tag{9}$$

where Λ is effectively the projection operator that causes this transition. By squaring this element, we'll get the probability. This may seem a bit vague but it will become much clearer when we start talking about time-dependent phenomena.

Let's do a little exercise now in which I'll stress the importance of these projections operators again. Suppose I have this function f and, whatever it is, I want to evaluate it at my observable A represented in a suitable basis. What can I do?

Whenever in doubt, expand in a power series. That's one of my top quotes by anyone on this planet. Fermi said that, and that's what we are going to do here. Suppose I pretend to expand my function f in a Taylor series but I'll do it in a vague manner, i.e. I'll absorb all the factors into a constant, c_j, and just focus on the expansion parameter, namely our operator, A:

$$f(A) = \sum_{j\geq 0} c_j A^j \tag{10}$$

Now, I want to express my operator in terms of *something*. That something will turn out to be its eigenvalues and eigenkets. Suppose I take my operator A and multiply it by 1:

$$A = A1 = A\left[\sum_n \Lambda_n\right] = A\sum_n |n\rangle\langle n| \tag{11}$$

Then I know how to act A on the ket:

$$A = \sum_n a_n |n\rangle\langle n| \tag{12}$$

This is called the *spectral decomposition* of an operator in terms of its eigenvalues and eigenkets. Let's take the powers of this operator:

$$A = \sum_n a_n |n\rangle\langle n| = \sum_n a_n \Lambda_n \tag{13}$$

$$A^2 = \left[\sum_n a_n |n\rangle\langle n|\right]\left[\sum_m a_m |m\rangle\langle m|\right] = \sum_n\sum_m a_n a_m |n\rangle \underbrace{\langle n|m\rangle}_{\delta_{nm}}\langle m| = \sum_n a_n^2 |n\rangle\langle n| = \sum_n a_n^2 \Lambda_n \tag{14}$$

or, let's use the properties of the projection operator:

$$A^3 = \left[\sum_n a_n \Lambda_n\right]\left[\sum_m a_m \Lambda_m\right]\left[\sum_k a_k \Lambda_k\right] = \sum_n\sum_m\sum_k a_n a_m a_k \underbrace{\underbrace{\Lambda_n \Lambda_m}_{\Lambda_n \delta_{nm}} \Lambda_k}_{\Lambda_n \delta_{nm}\delta_{nk}} = \sum_n a_n^3 \Lambda_n = \sum_n a_n^3 \Lambda_n \tag{15}$$

So we get the idea:

$$A^j = \sum_n a_n^j \Lambda_n \tag{16}$$

With this, our series expansion becomes

$$f(A) = \sum_{j\geq 0} c_j \left[\sum_n a_n^j \Lambda_n\right] = \sum_n \left[\sum_{j\geq 0} c_j a_n^j\right] \Lambda_n = \sum_n f(a_n)\Lambda_n \tag{17}$$

This way, we generalize the spectral decomposition into any functional form. Now, we don't need to worry about the operator itself. We just deal with the projections, which are easier to work with.

* * *

Now let's do an example about representations and measurements. Suppose I give you an observable A with the following properties:

$$\langle 1|A|1\rangle = a \tag{18}$$

$$\langle 1|A|2\rangle = b \tag{19}$$

$$\langle 2|A|1\rangle = b \tag{20}$$

$$\langle 2|A|2\rangle = a \tag{21}$$

Then, I give you a general state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle + i|2\rangle\right) \tag{22}$$

The question is, what are the probabilities that if I measure A on this state (say, the energy or the spin or any other observable if you want to leave this abstract realm), I get a, b, $a+b$, $a-b$ (in separate measurements, not within the same measurement)?

$$* * *$$

Measurement is nothing but taking projections. Using the projection operator and just the very basic assumptions about a measurement, Schwinger created a *measurement formalism* of quantum mechanics, which turned out to be identical to Schrödinger's wavefunction approach and Heisenberg's matrix mechanics.

We start with the *spectrum* of this operator A. Here, spectrum is just a fancy way of saying its eigenvalues and eigenstates. At this point, we are going to resort to matrices because it is highly convenient.

Now, we are given the A *sandwiches* above. What do we do with them? They appear to be the matrix elements of the operator A in the $\{|1\rangle, |2\rangle\}$ basis. So we may write

$$A \doteq \begin{pmatrix} a & b \\ b & a \end{pmatrix} \tag{23}$$

where $\doteq$ is read *can be represented by*. I just put a in the $(1,1)$ and $(2,2)$ entries and b in the $(1,2)$ and $(2,1)$ entries. How did I do that? This is a step that's usually taken without saying but it's crucial to be aware of that. We have tacitly assumed the representations

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{24}$$

Why? Because it's convenient. Now, I want to obtain the eigenvalues and the eigenvectors of this matrix. Let's use Mathematica [3].

```
A = {
    {a, b},
    {b, a}
};
```

Mathematica is row-major, so we enter the components row by row as we write them on paper. The newlines and the spacing that I'm using here are totally optional. Note the semicolon at the end. It just suppresses the output if you are working with a Mathematica notebook. Let's now play with this.

```
EigenValues[A]
EigenVectors[A]
```

When you evaluate this, the first output should be like

```
{a - b, a + b}
```

and the second output is

```
{{-1, 1}, {1, 1}}
```

So the eigenvalues are

$$\lambda_{\pm} = a \pm b \tag{25}$$

The unnormalized eigenvector corresponding to the *plus* eigenvalue is

$$|\widetilde{+}\rangle \doteq \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{26}$$

and the unnormalized eigenvector corresponding to the *minus* eigenvalue is

$$|\widetilde{-}\rangle \doteq \begin{pmatrix} -1 \\ 1 \end{pmatrix} \tag{27}$$

I'm going to normalize the *plus* eigenket by $1/\sqrt{2}$ and the *minus* eigenket by $-1/\sqrt{2}$. There is nothing that prevents me from choosing some other factor—even a complex one—but this is what I like. So, the normalized eigenkets are

$$|\pm\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \tag{28}$$

But remember these are just representations. We don't want to work with representations because they are just tools. Let's express the eigenkets in the basis $\{|1\rangle, |2\rangle\}$—even though they look abstract, it's these states that are our reality:

$$|\pm\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \pm \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}|1\rangle \pm \frac{1}{\sqrt{2}}|2\rangle = \frac{|1\rangle \pm |2\rangle}{\sqrt{2}} \tag{29}$$

With this, let's perform a spectral decomposition of the observable A:

$$\begin{aligned} A &= \sum_n a_n |n\rangle\langle n| \\ &= (a+b)|+\rangle\langle +| + (a-b)|-\rangle\langle -| \end{aligned} \tag{30}$$

where the projection operator to the *plus* eigenstate is given by

$$\Lambda_+ = |+\rangle\langle +| = \frac{|1\rangle + |2\rangle}{\sqrt{2}} \frac{\langle 1| + \langle 2|}{\sqrt{2}} \tag{31}$$

and the projection operator to the *minus* eigenstate is given by

$$\Lambda_- = |-\rangle\langle -| = \frac{|1\rangle - |2\rangle}{\sqrt{2}} \frac{\langle 1| - \langle 2|}{\sqrt{2}} \tag{32}$$

Finally, let's do some measurement. The spectral decomposition tells you what you can get if you try to measure the observable A on any state. You can either get $a+b$ or $a-b$. There is no other possibility. In a way, you can only measure that is in your spectrum [4]. Therefore, without doing any other calculation, we can directly conclude that the probability of measuring A to be a or b on any state is 0.

We can get $a+b$ and $a-b$, so let compute the probability amplitudes. We have

$$\Lambda_+|\psi\rangle = \frac{|1\rangle + |2\rangle}{\sqrt{2}} \frac{\langle 1| + \langle 2|}{\sqrt{2}} \frac{|1\rangle + i|2\rangle}{\sqrt{2}} \tag{33}$$

Noting that $\langle 1|2\rangle = 0$ and $\langle 1|1\rangle = \langle 2|2\rangle = 1$ (because that's how we chose these basis vectors), we get

$$\Lambda_+|\psi\rangle = |+\rangle \frac{1+i}{2} \tag{34}$$

so the probability of measuring A to be $a+b$ is

$$P(a+b) = \left|\frac{1+i}{2}\right|^2 = \frac{1}{2} \tag{35}$$

It is just a cute exercise of taking the inner product of 1's and 2's to show that measuring A to be $a-b$ has the same probability (so that the total probability is 1).

---

[1] This is true in the absence of degeneracies. When we have degeneracies, we say that the eigenvectors corresponding to the nondegenerate subset are orthogonal.

[2] Suppose we are working in an infinite-dimensional basis.

[3] To get a copy of Mathematica, go to https://www.it.northwestern.edu/software/mathematica-fac/index.html and click Students Wolfram Activation Key Request Form site under Activation and Download.

[4] But when you perform lots of measurement, your *average* may be some other value, depending on your state.