NOTES ON QUANTUM MECHANICS

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The purpose of these notes is to give a quick introduction to the mathematics behind quantum mechanics. Of all applications of the linear algebra we have been covering, perhaps none is so elegant and powerful as this. Of course, I am probably biased, but I still find this to be an amazing use of abstract vector spaces and linear operators which brings together many different concepts from this course. A background in physics will be useful, but is not required.

Mechanics is concerned with the behavior of physical systems over time. For instance, in the simplest example, we wish to describe the motion of a particle moving in a straight line from point A to point B. In classical mechanics, the state of the particle would be given by a real number, which is the position of the particle along the line segment from A to B. Similarly, for two-dimensional motion, the state is given by a point in a plane, and so on. Physical quantities like position and speed are measure by functions — evaluating the function representing speed on the state representing the particle simply gives the speed of the particle. The point is that all these physical quantities can all be measured exactly, and we can obtain a complete description of our physical system.

In quantum mechanics, it is no longer possible to have a complete, exact description of a physical system as above. The main difference is that we cannot talk about the exact state a system is in, but only about the *probability* that it will be in a given state. This reliance on probabilities is what makes quantum mechanics so strange, and yet we will see that linear algebra forces us to only be able to describe probabilities and not exact measurements. Let's get started!

The state of a physical system in quantum mechanics is given by a vector in a vector space V, called the *state space* of the system. For simplicity, say we have a particle moving on the interval $[0, 1]$. The state space is then (almost) the vector space of infinitely differentiable functions on $[0, 1]$ which vanish to all orders at 0 and 1:

$$H = \{f \in C^\infty([0, 1]) \mid f^{(k)}(0) = f^{(k)}(1) = 0 \text{ for all } k\}.$$

Actually, the state space is larger than this, but this is a good enough approximation. Indeed, we will only be using this as an example to illustrate some concepts we will talk about, so it's not crucial that you fully understand this vector space. The element $f \in H$ representing a physical system is what is called the *wave function* of the system.

So, states are described by elements of a vector space. What describes physical quantities such as position and speed? Operators! Indeed, each physical quantity corresponds to an operator on the state space V. In the example H above, position corresponds to the operator M which is multiplication by x, and speed corresponds to the operator D which is differentiation. Don't worry about why this is so — the reasons for the use of these operators goes way beyond the scope of this course.

Given an operator T on V representing a physical quantity, how do we measure the physical values associated with T? For example, how do we extract position and speed from the above operators? It turns out that the actual physical results achieved as the result of a measurement are the eigenvalues of the operator. So, the actual measurements you can get for the physical

quantity represented by the operator T are exactly the eigenvalues of T. A state vector e which is an eigenvector for an eigenvalue λ of T:

$$Te = \lambda e,$$

is called an *eigenstate* of T.

To summarize so far:

- States of a physical system are given by vectors in a vector space,
- Measurable physical quantities are given by operators,
- Possible results of actual measurements are given by eigenvalues.

Now we introduce probabilities. For this, we will need an inner-product on our space, so that the state space V is actually an inner-product space. For the H given before, the inner product is the usual one:

$$\langle f, g\rangle = \int_0^1 f(x)g(x)\,dx.$$

Notice that if we want to interpret actual results of measurements as eigenvalues of operators, we should require that our operators actually have eigenvalues. To guarantee this, we will actually assume that our operators our self-adjoint with respect to the given inner-product. The Spectral Theorem will then imply we have all the eigenvalues (and eigenvectors) we need.

For our example H, the multiplication operator M is self-adjoint, but the differentiation operator D is not — in fact, we saw in class that the integration by parts formula implies that D is *skew-adjoint*, meaning $D^* = -D$. However, for any skew-adjoint operator, multiplication by i gives a self-adjoint operator, so iD is self-adjoint. Hence in reality, the speed operator should be iD and not just D — we will ignore this minor point here. This procedure for constructing self-adjoint operators is the main reason why complex numbers show up all over the place in quantum mechanics.

The Spectral Theorem gives an orthonormal basis $(e_1, \ldots, e_n)$ of our state space V where each basis vector is an eigenstate of T; let $(\lambda_1, \ldots, \lambda_n)$ denote the corresponding eigenvalues. As we have seen in cass, the main point of the Spectral Theorem is that it gives a way to describe the full operator T in terms of the simpler data of the eigenvectors and eigenvalues.

Now, given a state vector v, we have

$$v = \langle v, e_1\rangle e_1 + \cdots + \langle v, e_n\rangle e_n.$$

Probabilities in quantum mechanics come from these inner products. In particular, the quantity

$$|\langle v, e_i\rangle|^2$$

is interpreted as the probability of finding your physical system (represented by the state vector v) to be in the state e_i. Hence we do not talk about the precise state a system will be in, but only the probability that it will be in a certain (eigen)state. The interpretation of the expression

$$Tv = \langle v, e_1\rangle \lambda_1 e_1 + \cdots + \langle v, e_n\rangle \lambda_n e_n$$

is that when attempting to measure the physical quantity represented by T on a state v, the result will be the value λ_i with probability $|\langle v, e_i\rangle|^2$. This is the key to the quantum mechanical description of physics.

Note that the probability of finding a state v to be in any eigenstate whatsoever should be 1 since we will always find the a state to be in some eigenstate when performing a measurement,

i.e. it is 100% likely that we will find some value as the result of performing a measurement. Thus, we should require that the total probability

$$|\langle v, e_1\rangle|^2 + \cdots + |\langle v, e_n\rangle|^2 = \|v\|^2$$

be 1, and hence that v have norm 1.

To (re)summarize, in a quantum mechanical description of a physical system:

- States of the physical system are given by vectors of norm 1 in an inner-product space,
- Measurable physical quantities are given by self-adjoint operators,
- Possible results of actual measurement are given by eigenvalues of the operators,
- For an operator T with orthonormal eigenbasis $(e_1, \ldots, e_n)$, the probability of getting an eigenvalue λ_i as the result of measuring the physical quantity represented by T on a state v is $|\langle v, e_i\rangle|^2$.

Congratulations, you now understand the mathematics behind quantum mechanics! Actually, as I'm sure those of you who have taken a course in quantum mechanics before can attest to, things get a lot more complicated than this. But the above summary is still essentially the mathematical foundation on which quantum mechanics is based.

Let us use this now to give the mathematical interpretation of one of the core assumptions in quantum mechanics: the *uncertainty principle*. This basic fact about quantum mechanics essentially states that it is not possible to know both the position and momentum (just think of speed if you've never seen the notion of momentum before) of a physical system at any given time — the closer you get to measuring the position, the farther away you get from knowing the momentum, and vice-versa. This is not due to having equipment which is not good enough to measure these two physical quantities simultaneously, it is a basic fact about the quantum mechanical nature of the system itself. Here's why.

As we've seen, measuring a physical quantity amounts to finding the eigenvalues of an operator. For self-adjoint operators, this amounts to finding a basis of eigenvectors. So, measuring a physical quantity amounts to diagonalizing an operator. To measure two physical quantities simultaneously requires that we find a basis which consists of common eigenvectors to the corresponding operators. In other words, two physical quantities can be simultaneously measured if and only if the corresponding self-adjoint operators are simultaneously diagonalizable. However, the last problem on the midterm (and the comments I made in the solution) show that two diagonalizable operators are simultaneously diagonalizable if and only if they commute. So finally, two physical quantities can be simultaneously measured if and only if the corresponding operators commute.

Recall the example H we had before, with the multiplication by x operator M representing position and the differentiation operator D (or more precisely iD) representing momentum (or speed in this simple case). Note that for any $f \in H$,

$$DM(f(x)) = D(xf(x)) = f(x) + xf'(x)$$

as follows from the product rule, and

$$MD(f(x)) = M(f'(x)) = xf'(x).$$

Thus $(DM - MD)(f(x)) = f(x) + xf'(x) - xf'(x) = f(x)$, so

$$DM - MD = \text{identity operator}.$$

This is not zero, so D and M do not commute, and hence are not simultaneously diagonalizable. Thus position and momentum cannot be simultaneously measured!

We thus have a mathematical reason as to why the uncertainty principle holds, which comes from the linear algebraic formulation of quantum mechanics. In particular, the uncertainty

principle is the source of the "weirdness" of quantum mechanics and is the source of the need to use probabilities. Thus, it is in this way that linear algebra really does fully describe the way the universe (at least quantum mechanically) works. Tada! :)