Notes on Quantum Mechanics: Formalism

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1 What These Notes Aim to Do

This is the first in a series of notes on Quantum Mechanics, where I work through texts by Shankar and Griffiths as well as 8.04 and 8.05 from MIT OpenCourseWare to learn Quantum Mechanics by myself. These notes are meant to reinforce and share my understanding of the material by actually producing some cohesive piece of writing. Now it would be a total nonsense if I just copied their words verbatim onto here, so instead I will be organizing their ideas into a fashion that I personally would find reasonable and understandable. I will also be abbreviating mathematical details that can easily be found online or in the literature when I feel like they are not too relevant (less so in this particular note). Quantum Mechanics is fascinating and is an introduction to the modern frontier of physics, and I hope that these notes will be a recapitulation of this amazing journey of mankinds' most brilliant minds.

2 Linear Operators as Matrices

It is a well-known result in linear algebra that if one knows how an operator transforms the basis vectors, then they will be able to determine completely how the operator will transform any vector in that basis.

Suppose that we have this transformation where an arbitrary linear operator A acts on a set of orthogonal vectors that form a basis in $\mathbf{R}^n$:

$$A|i\rangle = |i'\rangle \in \mathbf{R}^n$$

We now effectively have a new basis that are formed by the $|i'\rangle$'s. Each vector in the new basis, however, can still be written as a linear combination of vectors in the old basis. With that in mind, let us now turn our attention to an arbitrary vector in the old basis:

$$|V\rangle = a_1|1\rangle + a_2|2\rangle + ... + a_n|n\rangle$$

After a transformation by A, $|V\rangle$ becomes

$$|V'\rangle = A|V\rangle = a_1|1'\rangle + a_2|2'\rangle + ... + a_n|n'\rangle$$

As mentioned above, this vector still has a representation in the old basis. So if we take the inner product of one of the original basis vectors with our new vector, we will get back the component of the new vector in the old basis:

$$\langle i|V'\rangle = \langle i|A|V\rangle = \sum_{j=1}^{n} a_j \langle i|A|j\rangle = a'_i \tag{1}$$

where I pulled the j out of the inner product. Equation (1) has a nice matrix representation:

$$\begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \\ a'_n \end{pmatrix} = \begin{pmatrix} \langle 1|A|1\rangle & \langle 1|A|2\rangle & \dots & \langle 1|A|n\rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle n|A|1\rangle & \langle n|A|2\rangle & \dots & \langle n|A|n\rangle \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \tag{2}$$

In a more concise form:

$$\begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \\ a'_n \end{pmatrix} = \begin{pmatrix} |1'_o\rangle & |2'_o\rangle & \dots & \langle|N'_o\rangle \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \tag{3}$$

where $|i'_o\rangle$ is the representation of $|i'\rangle$ in the original basis. We can therefore define the matrix to be the representation of the operator in that basis:

$$A = \begin{pmatrix} \langle 1|A|1\rangle & \langle 1|A|2\rangle & \dots & \langle 1|A|n\rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle n|A|1\rangle & \langle n|A|2\rangle & \dots & \langle n|A|n\rangle \end{pmatrix} = \begin{pmatrix} |1'_o\rangle & |2'_o\rangle & \dots & \langle|N'_o\rangle \end{pmatrix} \tag{4}$$

Having a matrix representation for an operator, we can now derive more useful results regarding operators. Let us first define the **projection operator**, as it will prove very useful to us. Consider an arbitrary vector expanded in some basis:

$$\begin{aligned} |V\rangle &= \sum_{i=1}^{n} v_i|i\rangle = \sum_{i=1}^{n}\langle i|V\rangle|i\rangle \\ &= \sum_{i=1}^{n} |i\rangle\langle i|V\rangle = \sum_{i=1}^{n}(|i\rangle\langle i|)|V\rangle \\ &\equiv \sum_{i=1}^{n} P_i|V\rangle \end{aligned}$$

So we have defined $|i\rangle\langle i|$ to be P_i. In words, $P_i|V\rangle$ gives you the i-th component *and* basis vector of V. Note that $|i\rangle\langle i|$ is an $n \times n$ matrix while $\langle i|i\rangle$ is just a number. This is allows us to define $|i\rangle\langle i|$ as an operator. The projection operator has the following property:

$$I = \sum_{i=1}^{n} P_i \tag{5}$$

since

$$|V\rangle = (\sum_{i=1}^{n} P_i)|V\rangle = I|V\rangle$$

where I used the fact that matrix multiplication is distributive in a single direction.

Now consider a product of operators A and B, the element in the i-th row and j-th column is:

$$(AB)_{ij} = \langle i|AB|j\rangle = \langle i|AIB|j\rangle = \sum_{k=1}^{n}\langle i|A|k\rangle\langle k|B|j\rangle$$

using our matrix representation as in Equation (4), we have that

$$(AB)_{ij} = \sum_{k=1}^{n} A_{ik}B_{kj}$$

This then implies that the product of two operators can be represented as the product of their matrices.

We now turn our attention towards a special kind of operators. Given that

$$(|aV\rangle)^* = \langle V|a^* = \langle aV|$$

we can define operators H and $H^\dagger$ in analogy:

$$(|HV\rangle)^* = \langle V|H^\dagger = \langle HV|$$

$H^\dagger$ is termed the **adjoint** or **Hermitian conjugate** of the operator H. In a given basis, the adjoint operation is identical to taking a complex conjugate. Furthermore, an operator is said to be **Hermitian** if $H^\dagger = H$. In a basis defined on $\mathbf{R}^n$, a Hermitian matrix is also called a **symmetric** matrix. Furthermore, if an operator U satisfies the condition that $U^\dagger U = UU^\dagger = I$, it is said to be **unitary**. In a basis defined on $\mathbf{R}^n$, a unitary matrix is also called a **orthogonal** matrix.

We now set out to prove some properties of unitary operators.

Lemma 2.1. *Transformations by unitary operators preserve inner products and thus length.*

Proof. Let U be an arbitrary unitary operator, $|A\rangle$ and $|B\rangle$ be an arbitrary vector in a given basis. Then we have that

$$\langle UA|UB\rangle = \langle A|U^\dagger U|B\rangle = \langle A|I|B\rangle = \langle A|B\rangle$$

□

Therefore, we see that an unitary operator is essentially a generalized rotation operator (to the complex numbers) since it preserves inner products, or "length" as we most commonly conceptualize them.

Lemma 2.2. *The product of two unitary operators is also unitary.*

Proof. Let A and B be two unitary operators. Then

$$(AB)(AB)^\dagger = ABB^\dagger A^\dagger = AIA^\dagger = AA^\dagger = I$$

□

Lemma 2.3. *The determinant of a unitary matrix is a complex number of unitary modulus.*

Proof. Let U be a unitary matrix, then

$$\begin{aligned}
\det(I) &= \det(U^\dagger U) \\
&= \det(U^\dagger)\det(U) \\
&= \det(U^T)^* \det(U) \\
&= \det(U)^* \det(U) \\
&= |\det(U)|^2 \\
1 &= |\det(U)|^2
\end{aligned}$$

where I used the fact that $\det(AB) = \det(A)\det(B)$ and $\det(A^T) = \det(A)$. □

Just for fun, I will also prove some results about traces of generalized matrices.

Lemma 2.4. *If A and B are two arbitary matrices, then $tr(AB) = tr(BA)$.*

Proof. $\mathrm{tr}(AB) =$ □

Lemma 2.5. *Traces of a product of matrices is invariant under a cyclic exchange, that is, $tr(ABC) = tr(CAB) = tr(BCA)$*

Proof. $\mathrm{tr}(AB) =$ □

Lemma 2.6. *If U is a unitary matrix, and A is an arbitary matrix, then $tr(U^\dagger AU) = Tr(A)$*

Proof. $\mathrm{tr}(AB) =$ □

3 The Eigenvalue Problem and Degeneracy

Having looked at the representation of operators as matrices, which makes it easier to work with operators and vectors, we now turn our attention towards a special class of operator-vector relations. In the most general scenario, an operator acts on a vector to turn it into another vector:

$$A|\omega\rangle = |\omega'\rangle$$

Sometimes, we get a special kind of operator-vector relation, in which the vector is simply rescaled by a scalar factor:

$$A|\omega\rangle = \omega|\omega\rangle$$

It would turn out to be the case that these scenarios lie at the heart of analysis of Quantum Mechanical objects. This can be called an **eigenvalue equation**, where $|\omega\rangle$ is an eigenvector of A with the eigenvalue ω. Following are several useful theorems regarding eigenvalues and eigenvectors that are not incredibly hard to prove.

Theorem 3.1. *Eigenvalues of a unitary operator are complex numbers with unit modulus.*

Theorem 3.2. *Eigenvectors of a unitary operator are mutually orthogonal to each other, assuming that there is no degeneracy. If there is degeneracy, it is still possible to construct a eigenbasis in which vectors are mutually orthogonal.*

Theorem 3.3. *Eigenvalues of a Hermitian operator are real.*

Theorem 3.4. *For any Hermitian operator H, it is possible to construct at least one orthonormal eigenbasis. In addition, H is a diagonal matrix in this basis with its eigenvalues on the diagonal.*

With Theorem 4.4 in mind, we can prove further useful results regarding Hermitian operators and their matrices. Let's say that our Hermitian Operator is given by a matrix in some orthonormal basis, as it usually is the case, since its eigenbasis is also orthonormal, there must be *some* unitary operator U that rotates the entire basis onto the eigenbasis:

$$U|i\rangle = |\omega_i\rangle$$

Under this change of basis to an eigenbasis, the elements of the operator H's matrix is changed in the following way:

$$\langle i|H|j\rangle \to \langle \omega_i|H|\omega_j\rangle = \langle Ui|H|Uj\rangle = \langle i|U^\dagger HU|j\rangle$$

That is, if all of its basis vectors were transformed into its eigenbasis vectors by U, a Hermitian operator H would undergo the following change:

$$H \to U^\dagger HU \equiv H_d$$

where as mentioned in Theorem 4.4, H_d is a diagonal matrix with H's eigenvalues on its diagonal. For this to be true, this condition must be satisfied: $HU = UH_d$. This implies that

$$\begin{aligned} HU &= H\begin{bmatrix}|u_1\rangle & |u_2\rangle & \dots & |u_n\rangle\end{bmatrix} = \begin{bmatrix}H|u_1\rangle & H|u_2\rangle & \dots & H|u_n\rangle\end{bmatrix} \\ &= UH_d = \begin{bmatrix}\omega_1|u_1\rangle & \omega_2|u_2\rangle & \dots & \omega_n|u_n\rangle\end{bmatrix} \end{aligned}$$

or

$$\begin{bmatrix}H|u_1\rangle & H|u_2\rangle & \dots & H|u_n\rangle\end{bmatrix} = \begin{bmatrix}\omega_1|u_1\rangle & \omega_2|u_2\rangle & \dots & \omega_n|u_n\rangle\end{bmatrix} \tag{6}$$

This means that U's columns are eigenvectors of H! In summary then, we come to the conlusion that *given a Hermitian operator H and its matrix, we can always construct a unitary matrix U with its normalized orthogonal eigenvectors such that $U^\dagger HU = H_d$, where H_d is a diagonal matrix with H's eigenvalues on its diagonal; furthermore, the order of these eigenvalues correspond to the order of the eigenvector columns in U.*

With the diagonal picture of Hermitian operators in mind, we can turn our attention towards functions of or involving operators, where we can loosely conceptualize them as special kinds of numbers that do not commute. We focus our attention on functions that can be easily written as a power series, such as:

$$f(x) = e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

With that in mind, let us examine the operator $U = e^{iH}$, where H is a Hermitian operator:

$$e^{iH} = \sum_{n=0}^{\infty} \frac{(iH)^n}{n!}$$

If we go to the eigenbasis of H, we can get it to become diagonal:

$$U = e^{iH} = \sum_{n=0}^{\infty} \frac{(iH)^n}{n!} = \sum_{n=0}^{\infty} \frac{i^n}{n!} \begin{pmatrix} \omega_1^n & 0 & \dots & 0 \\ 0 & \omega_2^n & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \omega_m^n \end{pmatrix}$$

similarly

$$U^\dagger = (e^{iH})^\dagger = \sum_{n=0}^{\infty} \frac{(i^n)^\dagger}{n!} \begin{pmatrix} \omega_1^n & 0 & \dots & 0 \\ 0 & \omega_2^n & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \omega_m^n \end{pmatrix}$$

With a quick analysis of the different possible cases, one can arrive at the conclusion that $(i^n)^\dagger = (-i)^n$. So we have that

$$U = \begin{pmatrix} \sum_{n=0}^{\infty} \frac{i^n \omega_1^n}{n!} & 0 & \dots & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{i^n \omega_2^n}{n!} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sum_{n=0}^{\infty} \frac{i^n \omega_m^n}{n!} \end{pmatrix} = \begin{pmatrix} e^{i\omega_1} & 0 & \dots & 0 \\ 0 & e^{i\omega_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & e^{i\omega_m} \end{pmatrix}$$

and that

$$U^\dagger = \begin{pmatrix} \sum_{n=0}^{\infty} \frac{(-i)^n \omega_1^n}{n!} & 0 & \dots & 0 \\ 0 & \sum_{n=0}^{\infty} \frac{(-i)^n \omega_2^n}{n!} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sum_{n=0}^{\infty} \frac{(-i)^n \omega_m^n}{n!} \end{pmatrix} = \begin{pmatrix} e^{-i\omega_1} & 0 & \dots & 0 \\ 0 & e^{-i\omega_2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & e^{-i\omega_m} \end{pmatrix}$$

Then it remains a trivial computation to see that $U^\dagger U = I$ and thus U is a unitary operator. This example gives an intuition as to how to make sense of operators that are used as if they are numbers in functions, and extends well to other functions that utilizes the same idea.

4 Infinite Dimensions and Hilbert Space

A function can be represented by a vector in the following way: sample a finite amount n of points in the function's domain, record their output values and put each one of them into a vector:

$$|f_n\rangle \to \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{pmatrix}$$

We can choose the basis to simply just be columns of the n-dimensional identity matrix. Note that we have now constructed an n-dimensional *vector space* to represent a function which is in its own coordinate system (x-y plane for instance). So that even if a function is defined in the 2-dimensional x-y plane, if we choose say like 200 points on its domain to sample, its corresponding vector representation will live in a 200-dimensional vector space. Along the i-th axis in this 200-dimensional vector space, we will have a vector with component $f(x_i)$. If we wanted a better representation, or even better — the perfect representation, we would have to let n go to infinity. On this new infinite-dimensional vector space, we can define the inner product of two functions to be an integral:

$$\lim_{n\to\infty}\langle f_n|g_n\rangle = \lim_{n\to\infty} f^*(x_1)g(x_1) + f^*(x_2)g(x_2) + ... + f^*(x_n)g(x_n) = \int_a^b f(x)^* g(x)\, dx$$

Where I have gone ahead and extended the functions to the complex plane. Now note that even though the basis vectors in this infinite vector space obey orthogonality in the sense that $\langle i|j\rangle = 0$ if $i \neq j$, it is *not* true that $\langle i|i\rangle = 1$ as a careful analysis will show. I will skip that part. In an infinite vector space, orthogonality works as follows:

$$\langle i|j\rangle = \delta(i-j)$$

where $\delta(i-j)$ is the **Dirac Delta Function**, which is not really a function but a distribution, defined as

$$\delta(i-j) = 0 \quad \text{if } i \neq j$$
$$\int \delta(i-j)\, di = 1$$

In Quantum Mechanics, we are primarily concerned with functions that are square integrable on some given interval (a,b):

$$\langle f|f\rangle < \infty$$

The set of all f's that satisfy this condition make up what is called the **Hilbert Space**. If a function lives outside the Hilbert Space, it is unlikely that it will be able to describe anything physical *by itself*. But as we will see later, it is possible to superimpose many non-square-integrable functions to obtain one that is; we call the entire collection of such non-square-integrable functions and square-integrable functions the *physical Hilbert Space* to avoid confusion.

How is the knowledge of eigenvalues and eigenvectors helpful for us? It turns out that one of the central postulates of QM — the Schrödinger Equation — often poses eigenvalue problems for us. To solve the equation, we can adhere to the following general steps:

1. Solve the eigenvalue problem (find the eigenvectors and eigenvalues!)
2. Now that your operator is represented by a diagonal matrix, the decoupled differential equations should be generally easy to solve. Solve them to obtain something called a **propagator**.
3. The propagator handles the time evolution of the initial states. The problem has now been completely solved.

We will clarify what a propagator is later. Furthermore, we will see examples of these procedures not just in QM, but in classical mechanics of oscillations as well!

This mathematical framework will be extended when we begin to solve the Schrödinger Equation in various scenarios. We will encounter especially interesting constructs such as the commutator and uncertainty relationships.