QUANTUM MECHANICS
A Quick Guide

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Preface

Greetings,

Quantum Mechanics, A Quick Guide to... is my reading notes from Shankar's *Principles of Quantum Mechanics, Second Edition.* Additional material will come from my class notes and my comments/interpretations/solutions.

A strong background in linear algebra will be very helpful. I will try to cover some of the mathematical background, but a lot of familiarity will be assumed.

Enjoy!

Contents

12 Rotational Invariance and Angular Momentum　　　　　　　**30**

13 The Hydrogen Atom　　　　　　　**31**

14 Spin　　　　　　　**32**

15 Additional of Angular Momentum　　　　　　　**33**

16 Variational and WKB Methods　　　　　　　**34**

17 Time-Independent Perturbation Theory　　　　　　　**35**

18 Time-Dependent Perturbation Theory　　　　　　　**36**

19 Scattering Theory　　　　　　　**37**

20 The Dirac Equation　　　　　　　**38**

21 Path Integrals–II　　　　　　　**39**

22 Selected Problems and Solutions　　　　　　　**40**

1 Mathematical Introduction

1.1 Linear Vector Spaces

We should familiar with defining characteristics of linear vector spaces at this point. Here are some important definitions/theorems again:

Definition 1.1. A linear vector space $\mathbf{V}$ is a collection of objects called *vectors* for which there exists

1. A definite rule for summing, and

2. A definite rule for scaling, with the following features:

   - Closed under addition: for $x, y \in \mathbf{V}$, $x + y \in \mathbf{V}$.
   - Closed under scalar multiplication: $x \in \mathbf{V}$, then $ax \in \mathbf{V}$ for some scalar a.
   - Scalar multiplication is distributive.
   - Scalar multiplication is associative.
   - Addition is commutative.
   - Addition is associative.
   - There exists a (unique) null element in $\mathbf{V}$.
   - There exists a (unique) additive inverse.

Vector spaces are defined over some field. The field can be real numbers, complex numbers, or it can also be finite. As for good practice, we will begin to label vectors with Dirac bra-ket notation. So, for instance, $|v\rangle \in \mathbf{V}$ denotes vector $v \in \mathbf{V}$. Basic manipulations of these vectors are intuitive:

1. $|0\rangle$ is unique, and is the null element.

2. $0 \, |V\rangle = |0\rangle$.

3. $|-V\rangle = -\, |V\rangle$.

4. $|-V\rangle$ is a unique additive inverse of $|V\rangle$.

The reasons for choosing to use the Dirac notation will become clear later on. Another important basic concept is *linear (in)dependence*. Of course, there are a number of equivalent statement for linear independence. We shall just give one here:

Definition 1.2. A set of vectors is said to be linearly independent if the only linear relation

$$\sum_{i=1}^{n} a_i \, |i\rangle = |0\rangle \tag{1}$$

is the trivial one where the components $a_i = 0$ for any i.

The next two basic concepts are *dimension* and *basis*.

Definition 1.3. A vector space $\mathbf{V}$ has dimension n if it can accommodate a maximum of n linearly independent vectors. We denote this n-dimensional vector space as $\mathbf{V}^n$.

We can show that

Theorem 1.1. Any vector $|v\rangle \in \mathbf{V}^n$ can be written (uniquely) as a linear combination of any n linearly independent vectors.

Definition 1.4. A set of n linearly independent vectors in a n-dimensional space is called a *basis*. So if $|1\rangle, \ldots, |n\rangle$ form a basis for $\mathbf{V}^n$, then any $|v\rangle \in \mathbf{V}$ can be written uniquely as

$$|v\rangle = \sum_{i=1}^{n} a_i |i\rangle. \tag{2}$$

It is nice to remember the following:

$$\boxed{\text{Linear Independence} = \text{Basis} + \text{Span}} \tag{3}$$

When a collection of vectors span a vector space $\mathbf{V}$, it just means that any $|v\rangle \in \mathbf{V}$ can be written as a linear combination of (some of) these vectors.

The algebra of linear combinations is quite intuitive. If $|v\rangle = \sum_i a_i |i\rangle$ and $|w\rangle = \sum_i b_i |i\rangle$ then

1. $|v + w\rangle = \sum_i (a_i + b_i) |i\rangle$.

2. $c |v\rangle = c \sum_i a_i |i\rangle = \sum_i c a_i |i\rangle$.

A linear algebra text will of course provide a much better coverage of these topics.

1.2 Inner Product Spaces

A generalization of the familiar dot product is the *inner product* or the *scalar product*. An inner product between two vectors $|v\rangle$ and $|w\rangle$ is denoted $\langle v|w|v|w\rangle$. An inner product has to satisfy the following properties:

1. Conjugate symmetry (or skew-symmetry):$\langle v|w\rangle = \langle w|v\rangle^*$.

2. Positive semi-definiteness: $\langle v|v\rangle \geq 0$.

3. Linearity in ket: $\langle v|aw + bz\rangle = a \langle v|w\rangle + b \langle v|z\rangle$.

4. Conjugate-linearity in bra: $\langle av + bz|w\rangle = \bar{a} \langle v|w\rangle + \bar{b} \langle z|w\rangle$.

Definition 1.5. An inner product space is a vector space with an inner product.

Definition 1.6. $\langle v|w \rangle = 0 \iff |v\rangle \perp |w\rangle$.

Definition 1.7. The *norm* (or length) of $|v\rangle$ is defined as

$$\|v\| = \sqrt{\langle v|v\rangle}. \tag{4}$$

Unit vectors have unit norm. Unit vectors are said to be *normalized*.

Definition 1.8. A set of basis vectors all of unit norm, which are pairwise orthogonal will be called an *orthonormal basis* or ONB.

Let $|v\rangle = \sum_i a_i |i\rangle$ and $|w\rangle = \sum_i b_i |j\rangle$, then

$$\langle v|w \rangle = \sum_i a_i^* b_i \langle i|j \rangle. \tag{5}$$

Theorem 1.2. Gram-Schmidt: Given a linearly independent basis, we can form linear combinations of the basis vectors to obtain an orthonormal basis.

Suppose that the Gram-Schmidt process gives us an ONB then we have

$$\langle i|j \rangle = \delta_{ij}. \tag{6}$$

As a result,

$$\langle v|w \rangle = \sum_i v_i^* w_i. \tag{7}$$

Alternatively, we can think this as doing the standard inner products of vectors whose entries are the components of the vectors $|v\rangle$, $|w\rangle$ in the basis:

$$|v\rangle \rightarrow \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} \quad |w\rangle \rightarrow \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} \implies \langle v|w \rangle = \begin{bmatrix} v_1^* & v_2^* & \dots & v_n^* \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}. \tag{8}$$

We can also easily see that

$$\langle v|v \rangle = \sum_i |v_i|^2 \geq 0. \tag{9}$$

1.3 Dual Spaces and Dirac Notation

Here we deal with some technical details involving the *ket* (the column vectors) and the *bra* (the row vectors). Column vectors are concrete manifestations of an abstract vector $|v\rangle$ in a basis, and we can work backward to go from the column vectors to the kets. We can do a similar thing with the bra vectors - since there's nothing special about writing the entries is a column versus in a row. However, we will do the following. We know that associated with every ket $|v\rangle$ is a column vector. So let its adjoint, which is a row vector, be associated with the bra, called $\langle v|$. Now, we have two vector spaces, the space of kets and the dual space of bras. There is a basis of vectors $|i\rangle$ for expanding kets and a similar basis $\langle i|$ for expanding bras.

1.3.1 Expansion of Vectors in an ONB

It is extremely useful for us to be able to express a vector in an ONB. Suppose we have a vector $|v\rangle$ in an ONB $|i\rangle$. Then, let $|v\rangle$ be written as

$$|v\rangle = \sum_i v_i \, |i\rangle. \tag{10}$$

To find the components v_i, we take the inner product of $|v\rangle$ with $|j\rangle$:

$$\langle j|v\rangle = \sum_i v_i \, \langle j|i\rangle = \sum_i v_i \delta_{ij} = v_j. \tag{11}$$

With this, we can rewrite the vector $|v\rangle$ in the basis $|i\rangle$ as

$$|v\rangle = \sum_i |i\rangle \, \langle i|v\rangle. \tag{12}$$

1.3.2 Adjoint Operations

Here is a few details regarding taking the adjoints of vectors. Suppose that

$$|v\rangle = \sum_i v_i \, |i\rangle = \sum_i |i\rangle \, \langle i|v\rangle. \tag{13}$$

Then,

$$\langle v| = \sum_i |i\rangle \, v_i^*. \tag{14}$$

Now, because $v_i = \langle i|v\rangle$, we have $v_i^* = \langle v|i\rangle$. Thus,

$$\langle v| = \sum_i \langle v|i\rangle \, \langle i|. \tag{15}$$

In plain words, the rule for taking the adjoint is the following. To take the adjoint of an equation involving bras and kets and coefficients, reverse the order of all factors, exchanging bras and kets and complex conjugating all coefficients.

1.3.3 Gram-Schmidt process

Again, the Gram-Schmidt process lets us convert a linearly independent basis into an orthonormal one. For a two-dimensional case, procedure is the following:

1. Rescale the first by its own length, so it becomes a unit vector. This is the first (orthonormal) unit vector.

2. Subtract from the second vector its projection along the first, leaving behind only the part perpendicular to the first. (Such a part will remain since by assumption the vectors are nonparallel).

3. Rescale the left over piece by its own length. We now have the second basis vector: it s orthogonal to the first and of unit length.

In general, let $|I\rangle, |II\rangle, \ldots$ be a linearly independent basis. The first vector of the orthonormal basis will be

$$|1\rangle = \frac{|I\rangle}{\||I\rangle\|}. \tag{16}$$

For the second vector in the basis, consider

$$|2'\rangle = |II\rangle - |1\rangle \langle 1|II\rangle. \tag{17}$$

We can see that $|2'\rangle$ is orthogonal to $|1\rangle$:

$$\langle 1|2'\rangle = \langle 1|II\rangle - \langle 1|1\rangle \langle 1|II\rangle = 0. \tag{18}$$

So dividing $|2'\rangle$ by its norm gives us, $|2\rangle$, the second element in the ONB. To find the third element in the ONB, we have to first make sure it is orthogonal to both $|I\rangle$ and $|II\rangle$, so let us consider

$$|3'\rangle = |III\rangle - |1\rangle \langle 1|III\rangle - |2\rangle \langle 2|III\rangle. \tag{19}$$

Once again we have $|3'\rangle$ orthogonal to both $|1\rangle$ and $|2\rangle$. Normalizing $|3'\rangle$ gives us $|3\rangle$, the third element in the ONB. We can now see how this process continues to the last element.

1.3.4 Schwarz and Triangle Inequality

Just two small yet very important details:

Theorem 1.3. Schwarz Inequality:

$$|\langle v|w\rangle| \leq \|v\|\|w\| \tag{20}$$

Theorem 1.4. Triangle Inequality:

$$\|v + w\| \leq \|v\| + \|w\|. \tag{21}$$

1.4 Subspaces, Sum and Direct Sum of Subspaces

I'm not too happy with the definitions given by Shankar's book. He also uses the notation for direct sum to indicate vector space addition, which is very confusing. Any linear algebra textbook would provide better definitions. For equivalent statements about directness of vector space sums, check out my Matrix Analysis notes.

1.5 Linear Operators

Again, a rigorous definition of an operator can be found in almost any linear algebra textbook. But here,we can simply think of an operator as just some linear transformation from a vector space to itself. Say, if Ω is some operator that sends $|v\rangle$ to $|v'\rangle$, we write

$$\Omega |v\rangle = |v'\rangle. \tag{22}$$

By definition, $|v\rangle$ and $|v'\rangle$ are contained in the same vector space. Now, we note that Ω can also act on bras:

$$\langle v| \Omega = \langle v'|. \tag{23}$$

But of course the order of writing things is different, and once again, $\langle v|$ and $\langle v'|$ are contained in the same (dual) space.

Next, because Ω is linear, we have the following familiar rules:

$$\Omega \alpha |v_i\rangle = \alpha \Omega |v_i\rangle. \tag{24}$$

$$\Omega\{\alpha |v_i\rangle + \beta |v_j\rangle\} = \alpha \Omega |v_i\rangle + \beta \Omega |v_j\rangle. \tag{25}$$

$$\langle v_i| \alpha \Omega = \langle v_i| \Omega \alpha \tag{26}$$

$$\{\langle v_i| \alpha + \langle v_j| \beta\}\Omega = \alpha \langle v_i| \Omega + \beta \langle v_j| \Omega. \tag{27}$$

One of the nice features of linear operators is that the action of an operator is completely determined by what it does to the basis vectors. Suppose

$$|v\rangle = \sum_i v_i |i\rangle \tag{28}$$

and

$$\Omega |i\rangle = |i'\rangle, \tag{29}$$

then

$$\Omega |v\rangle = \sum_i \Omega v_i |i\rangle = \sum_i v_i \Omega |i\rangle = \sum_i v_i |i'\rangle. \tag{30}$$

The next point of interest is *products* of operators. As we might have seen, operators don't always commute. A product of operators applied to a vector just means operators are applied in sequence. The *commutator* of two operators Ω, Λ is defined as

$$\Omega\Lambda - \Lambda\Omega \equiv [\Omega, \Lambda]. \tag{31}$$

In general, $[\Omega, \Lambda]$ is not zero. Suppose three operators Ω, Λ, Θ are involved, then we have two useful relations:

$$[\Omega, \Lambda\Theta] = \Lambda [\Omega, \Theta] + [\Omega, \Lambda] \Theta \tag{32}$$

$$[\Lambda\Omega, \Theta] = \Lambda [\Omega, \Theta] + [\Lambda, \Theta] \Omega. \tag{33}$$

We notice that the form resembles the chain rule in calculus.

1.6 Matrix Elements of Linear Operators

One thing we will hear very often in quantum mechanics is the idea of matrix elements. The idea, it turns out, is very simple. Suppose we have a basis $|i\rangle$, and an operator Ω such that

$$\Omega |i\rangle = |i'\rangle. \tag{34}$$

Then, for

$$|v\rangle = \sum_i v_i |i\rangle, \tag{35}$$

we have

$$\Omega |v\rangle = \Omega \sum_i v_i |i\rangle = \sum_i v_i \Omega |i\rangle = \sum_i v_i |i'\rangle. \tag{36}$$

Because we know Ω and $|i\rangle$, $|i'\rangle$ is also known, as in its components in the basis $|j\rangle$ (un-primed) are known:

$$\langle j|i'\rangle = \langle j| \Omega |i\rangle \equiv \Omega_{ji}, \tag{37}$$

where the n^2 numbers Ω_{ji} are the matrix elements of Ω in this basis. Now, if

$$\Omega |v\rangle = |v'\rangle \tag{38}$$

then the components of the transformed ket $|v'\rangle$ can be expressed in terms of the components of $|v\rangle$ and the matrix elements Ω_{ji}:

$$v_i' = \langle i|v'\rangle = \langle i| \Omega |v\rangle = \langle i| \Omega \sum_j v_j |j\rangle = \sum_j v_j \langle i| \Omega |j\rangle = \sum_j \Omega_{ij} v_j. \tag{39}$$

We can see the above equation in matrix form as well:

$$\begin{bmatrix} v_1' \\ \vdots \\ v_n' \end{bmatrix} = \begin{bmatrix} \langle 1| \Omega |1\rangle & \dots & \langle 1| \Omega |n\rangle \\ \vdots & \ddots & \vdots \\ \langle n| \Omega |1\rangle & \dots & \langle n| \Omega |n\rangle \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}. \tag{40}$$

The elements of the first column are simply the components of the first transformed basis vector $|1'\rangle = \Omega |1\rangle$ in the given basis. Likewise, the elements of the jth column represent the image of the jth basis vector after Ω acts on it.

1.7 Matrix Elements of Products of Operators

To get the matrix elements of a product of two operators, we do the following. Suppose we have operators Ω and Λ, then

$$(\Omega\Lambda)_{ij} = \langle i| \Omega\Lambda |j\rangle = \langle i| \Omega \mathcal{I} \Lambda |j\rangle. \tag{41}$$

Now, we observe that

$$\mathcal{I} = \sum_k |k\rangle \langle k| . \tag{42}$$

So,

$$(\Omega\Lambda)_{ij} = \sum_k \langle i| \Omega |k\rangle \langle k| \Lambda |j\rangle = \sum_k \Omega_{ik}\Lambda_{kj}. \tag{43}$$

1.8 The Adjoint of an Operator

Recall that for a scalar α

$$\langle \alpha v| = \langle v| \alpha^*, \tag{44}$$

then we have a similar thing with operators if

$$\Omega |v\rangle = |v'\rangle \tag{45}$$

then

$$\langle \Omega v| = \langle v| \Omega^\dagger, \tag{46}$$

where $\Omega^\dagger$ is *the* adjoint of Ω. The relationship between $\Omega^\dagger$ and Ω can be seen in a basis. We consider the matrix elements of $\Omega^\dagger$ in a basis:

$$(\Omega^\dagger)_{ij} = \langle i| \Omega^\dagger |j\rangle = \langle \Omega i|j\rangle = \langle j|\Omega i\rangle^* = \langle j| \Omega |i\rangle^* = \Omega_{ji}^*. \tag{47}$$

We see that

$$\Omega_{ij}^\dagger = \Omega_{ji}^*, \tag{48}$$

i.e., in matrix form, $\Omega^\dagger$ is the conjugate transpose of Ω.

The rule for taking adjoins of equations is rather simple: When a product of operators, bras, kets, ad explicit numerical coefficients is encountered, reverse the order of all factors and make the substitution $\Omega \leftrightarrow \Omega^\dagger$, $|\rangle \leftrightarrow \langle|$, $a \leftrightarrow a^*$.

1.9 Hermitian, Anti-Hermitian, and Unitary Operators

Definition 1.9. An operator Ω is Hermitian $\iff \Omega = \Omega^\dagger$.

Definition 1.10. An operator Ω is anti-Hermitian $\iff \Omega = -\Omega^\dagger$.

Shankar's book ignores a bigger class of operators called *normal* operators. Normal operators commute with their adjoints. In a sense, normal operators act *like numbers*. Hermitian (or self-adjoint) operators are a subset of normal operators. So, the number-likeness of normal operators carries over to Hermitian operators and anti-Hermitian operators as well. Hermitian and anti-Hermitian operators are like pure real and pure imaginary numbers. Just as every number

maybe be decomposed into a sum of pure real and pure imaginary parts, it turns out that we can decompose every operator into its Hermitian and anti-Hermitian parts.

$$\Omega = \frac{\Omega + \Omega^\dagger}{2} + \frac{\Omega - \Omega^\dagger}{2}. \tag{49}$$

One can verify that the first terms is Hermitian, and the second term is anti-Hermitian.

Definition 1.11. An operator $\mathcal{U}$ is unitary $\iff \mathcal{U}\mathcal{U}^\dagger = \mathcal{I}$.

Unitary operators are like complex numbers of unit modulus.

Theorem 1.5. Unitary operators preserves the inner product between the vectors they act on.

Proof. Suppose

$$|v'\rangle = \mathcal{U} |v\rangle \tag{50}$$
$$|w'\rangle = \mathcal{U} |w\rangle . \tag{51}$$

Then

$$\langle v'|w'\rangle = \langle \mathcal{U}v|\mathcal{U}w\rangle = \langle v| \mathcal{U}^\dagger \mathcal{U} |w\rangle = \langle v|w\rangle . \tag{52}$$

$\square$

Theorem 1.6. The columns (or rows) of a unitary matrix form an ONB.

Proof. Refer to a linear algebra text. The key is to consider an inner product between any two columns/rows. $\square$

1.10   Active and Passive Transformation

Suppose all $|v\rangle$ is unitarily transformed to $|v'\rangle$:

$$|v\rangle \to \mathcal{U} |v\rangle . \tag{53}$$

Then under this transformation, the matrix elements of any operator Ω are modified as follows:

$$|v'\rangle \Omega |v\rangle \to |\mathcal{U}v'\rangle \Omega |\mathcal{U}v\rangle = \langle v'| \mathcal{U}^\dagger \Omega \mathcal{U} |v\rangle . \tag{54}$$

It is clear that the same change is equivalent to leaving the vectors alone and subjecting all operators to the change

$$\Omega \to \mathcal{U}^\dagger \Omega \mathcal{U}. \tag{55}$$

Active transformation refers to changing the vectors, while *passive transformation* refers to changing the operators.

1.11 The Eigenvalue Problem

I won't say much about what eigenvectors and eigenvalues are because we should be familiar with these concepts at this point. But just to introduce some terminology, each operator has certain kets of its own called *eigenkets*, on which its action is simply that of scaling. So, eigenkets are just a different word for eigenvectors of an operator:

$$\Omega \left| v \right\rangle = \omega \left| v \right\rangle . \tag{56}$$

Shankar's book talks about the characteristic equation and characteristic polynomial. While these are legitimate ways to find eigenvalues and eigenvectors, it is often very difficult. I'd prefer Leo Livshits' and Sheldon Axler's way and use minimal polynomials instead. I would steer away from determinants and characteristic polynomials at this point.

Theorem 1.7. Eigenvalues of a Hermitian operator are real.

Proof. Suppose

$$\Omega \left| w \right\rangle = a \left| w \right\rangle , \tag{57}$$

then

$$\left\langle w \right| \Omega \left| w \right\rangle = a \left\langle w | w \right\rangle , \tag{58}$$

and thus

$$a^* \left\langle w | w \right\rangle = \left\langle w \right| \Omega^\dagger \left| w \right\rangle = \left\langle w \right| \Omega \left| w \right\rangle = a \left\langle w | w \right\rangle . \tag{59}$$

So we have

$$(a - a^*) \left\langle w | w \right\rangle = 0. \tag{60}$$

Because $\left| w \right\rangle$ are eigenkets, they are cannot be the zero vector. This means $a = a^*$. $\qquad\square$

Some might worry about the existence of eigenvalues of Hermitian operators. But worry no more, because Hermitian operators are a subclass of normal operators, which are a subclass of diagonalizable operators. This simply says Hermitian matrices are diagonalizable, and all its eigenvalues are real. But it turns out there is a little bit more to this.

Theorem 1.8. For every Hermitian operator Ω, there exists an ONB comprised entirely of the eigenvectors of Ω.

Once again, this should be no surprise if one has studied normal operators. Hermitian operators inherit this property from its normalness. This property of normal operators are called the Spectral Theorem (for normal operators, of course). The proof of all this can be found in many linear algebra texts.

Theorem 1.9. The eigenvalues of a unitary operator are complex numbers of unit modulus.

Proof. The key to the proof is using inner products. $\qquad\square$

1.11.1 Simultaneous Diagonalization of Two Hermitian Operators

I would say the topic of simultaneous diagonalizability is covered quite well in Leo Livshits' course and hence in my Matrix Analysis notes. But here I will just give the most important results.

Theorem 1.10. If Ω and Λ are two commuting Hermitian operators, there exists a basis of common eigenvectors that diagonalizes them both.

This result is not too surprising if we have studied simultaneous diagonalizability before. A more general theorem says that

$$\text{Simultaneous diagonalizbility} \iff \text{Individual diagonalizability} + \text{Commutativity.} \tag{61}$$

It is clear that because all Hermitian operators are diagonalizable, if two Hermitian operators commute, they are simultaneously diagonalizable.

1.11.2 The Propagator

In quantum mechanics (and classical mechanics of course), it is quite common to have some final state vector be obtained from an initial state vector multiplied by some matrix, which is independent of the initial state. We call this matrix the *propagator*.

The central problem in quantum mechanics is finding the state of a quantum system $|\psi\rangle$, which obeys the Schrödinger equation:

$$i\hbar \left|\dot{\psi}\right\rangle = J |\psi\rangle \tag{62}$$

where the Hermitian operator H is called the *Hamiltonian*. We will see much more of this as we move on.

1.12 Functions of Operators and Related Concepts

In this section, we look at whether it makes sense to define functions of operators. We will only restrict ourselves to functions that can be written as a power series. Consider a series

$$f(x) = \sum_{n=0}^{\infty} = a_n x^n \tag{63}$$

where x is a scalar. We defined the same function of an operator to be

$$f(\Omega) = \sum_{n=0}^{\infty} a_n \Omega^n. \tag{64}$$

Now, this definition only makes sense if we have convergence. Consider this example:

$$e^{\Omega} = \sum_{n=0}^{\infty} \frac{\Omega^n}{n!}, \tag{65}$$

where Ω is Hermitian. In the eigenbasis of Ω, Ω is diagonal. This means we can add and/or take powers of Ω by add and/or take powers of the diagonal entries. We can find that

$$e^\Omega = \begin{bmatrix} \sum_{m=0}^\infty \frac{\omega_1^m}{m!} & \\ & \sum_{m=0}^\infty \frac{\omega_n^m}{m!} \end{bmatrix} \tag{66}$$

where ω_i are the eigenvalues of Ω. We note that each entry in the expression above converges to e^{ω_i}.

1.12.1   Derivatives of Operators with Respect to Parameters

Now, consider some operator $\Theta(\lambda)$ that depends on a parameter λ. The derivative of Θ with respect to λ is defined to be

$$\frac{d\Theta(\lambda)}{d\lambda} = \lim_{\Delta\lambda \to 0} \left[\frac{\Theta(\lambda + \Delta\lambda) - \Theta(\lambda)}{\Delta\lambda} \right]. \tag{67}$$

If $\Theta(\lambda)$ is written as a matrix, then the matrix of $d\Theta/d\lambda$ is obtained by differentiating the matrix elements of $\Theta(\lambda)$. A case that might be interesting to us is

$$\Theta(\lambda) = e^{\lambda\Omega}. \tag{68}$$

It turns out that if Ω is Hermitian or "nice enough" then

$$\frac{d\Theta(\lambda)}{d\lambda} = \Omega e^{\lambda\Omega} = e^{\lambda\Omega}\Omega = \Theta(\lambda)\Omega = \Omega\Theta(\lambda). \tag{69}$$

Conversely, if we have

$$\frac{d\Theta(\lambda)}{d\lambda} = \Theta(\lambda)\Omega \tag{70}$$

then

$$\Theta(\lambda) = ce^{\lambda\Omega} \tag{71}$$

where c is some operator. But we have to be careful that c might not commute with $e^{\lambda\Omega}$.

The business of whether two operators commute or don't can make things slightly more complicated. If Θ and Ω commute, i.e., $[\Theta, \Omega] = 0$, then the rules of exponentiation carries over very nicely:

$$e^{a\Omega}e^{b\Omega} = e^{(a+b)\Omega} \tag{72}$$

$$e^{a\Omega}e^{b\Theta} = e^{a\Omega+b\Theta} \tag{73}$$

$$e^{a\Omega}e^{b\Theta}e^{-a\Omega} = e^{b\Theta}. \tag{74}$$

15

If $[\Omega, \Theta] \neq 0$, then the second and third equations no longer hold. Likewise, in differentiating a product, we have to be extra careful:

$$\frac{d}{d\lambda} e^{\lambda\Omega} e^{\lambda\Theta} = \Omega e^{\lambda\Omega} e^{\lambda\Theta} + e^{\lambda\Omega} e^{\lambda\Theta} \Theta. \tag{75}$$

While $[\Omega, e^{\lambda\Omega}] = 0$, because Θ and Ω might not commute, we can't bring Ω over to the right of $e^{\lambda\Theta}$.

1.13 Generalization to Infinite Dimensions

1.13.1 The Dirac delta function

Consider the ordered n-tuple $\{f_n(x_1), \ldots, f_n(x_n)\}$ as components of a ket $|f_n\rangle$ in a vector space $\mathbf{V}^n(\mathbb{R})$:

$$|f_n\rangle \leftrightarrow \begin{bmatrix} f_n(x_1) \\ \vdots \\ f_n(x_n) \end{bmatrix}. \tag{76}$$

The basis vectors in this space are:

$$|x_i\rangle \leftrightarrow \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow i^{th} \text{place}. \tag{77}$$

The basis vectors satisfy *orthogonality* and *completeness*:

$$\langle x_i | x_j \rangle = \delta_{ij} \tag{78}$$

$$\sum_{i=1}^n |x_i\rangle \langle x_i| = \mathcal{I}. \tag{79}$$

With this,

$$|f_n\rangle = \sum_{i=1}^n f_n(x_i) |x_i\rangle. \tag{80}$$

We next define the inner product in this space:

$$\langle f_n | g_n \rangle \ sum_{i=1}^n f_n(x_i) g_n(x_i). \tag{81}$$

16

The functions f_n and g_n are said to be orthogonal if $\langle f_n | g_n \rangle = 0$. We also have that

$$\langle f_n | f_n \rangle = \sum_{i=1}^{n} [f_n(x_i)]^2. \tag{82}$$

For finite n, nothing "bad" can really happen here. But what if n is infinity? What we need is the redefinition of the inner product for finite n in such a way that as n goes to infinity, we get a smooth limit. A natural choice is

$$\langle f_n | g_n \rangle = \sum_{i=1}^{n} f_n(x_i) g_n(x_i) \frac{L}{n+1} \tag{83}$$

where L is the length of the interval. If we now let n go to infinity, we get

$$\langle f | g \rangle = \int_0^L f(x) g(x) \, dx \tag{84}$$

$$\langle f | f \rangle = \int_0^L f^2(x) \, dx. \tag{85}$$

Now, if we consider complex functions as well in some interval $a \le x \le b$, the inner product becomes:

$$\langle f | g \rangle = \int_a^b f^*(x) g(x) \, dx. \tag{86}$$

But what are the basis vectors in this space and are they normalized? We know that

$$\langle x | x' \rangle = 0 \tag{87}$$

if $x \ne x'$. But what if $x = x'$? It turns out that we cannot simply require $\langle x | x \rangle = 1$. The best way to see this is to deduce the correct normalization. We start with the completeness relation:

$$\int_a^b |x'\rangle \langle x'| \, dx' = \mathcal{I}. \tag{88}$$

Now, consider this

$$\int_a^b \langle x | x' \rangle \langle x' | f \rangle \, dx' = \langle x | \mathcal{I} | f \rangle = \langle x | f \rangle. \tag{89}$$

This is nothing but the projection of $|f\rangle$ along the basis ket $|x\rangle$, which is just $f(x)$. So, we also have $f(x') = \langle x' | f \rangle$. Let the inner product $\langle x | x' \rangle$ be some unknown function $\delta(x, x')$. Since $\delta(x, x')$ vanishes if $x \ne x'$, we can restrict the

integral to an infinitesimal region near $x' = x$. With these, the equality above gives

$$\int_{x-\epsilon}^{x+\epsilon} \delta(x, x') f(x') \, dx' = f(x). \tag{90}$$

In this infinitesimal region, $f(x)$ can assumed to be constant, and thus can be pulled out of the integral, leaving

$$f(x) \int_{x-\epsilon}^{x+\epsilon} \delta(x, x') \, dx' = f(x). \tag{91}$$

And so we have

$$\int_{x-\epsilon}^{x+\epsilon} \delta(x, x') \, dx' = 1. \tag{92}$$

Clearly, $\delta(x, x')$ cannot be finite at $x = x'$. It should be infinite in such a way that its integral is 1. Since $\delta(x, x')$ depends only on the difference $x - x'$, we can write it as $\delta(x - x')$. So, the function $\delta(x - x')$ has the properties:

$$\begin{cases} \delta(x - x') = 0, & x \neq x' \\ \int_a^b \delta(x - x') \, dx' = 1 & a < x < b \end{cases}. \tag{93}$$

This is called the **Dirac delta function** and it fixes the normalization of the basis vectors:

$$\langle x | x' \rangle = \delta(x - x'). \tag{94}$$

The Dirac delta function is "strange" in the sense that its value is either zero or infinite. It's thus useful to view it as the limit of a Gaussian:
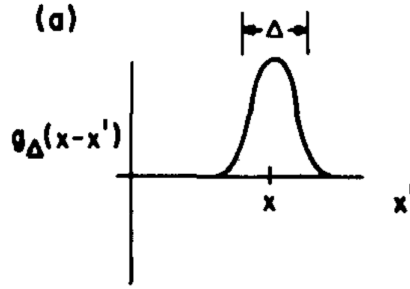
of the form

$$g_\Delta(x - x') = \frac{1}{\sqrt{\pi \Delta^2}} e^{-(x-x')^2/\Delta^2}. \tag{95}$$

It is clear that the area under the curve is one (one can easily check this). Also, $\Delta \to 0$, g_Δ becomes closer and closer to $\delta(x - x')$ (the area under the curve is the same, while the width of the peak becomes smaller and smaller).
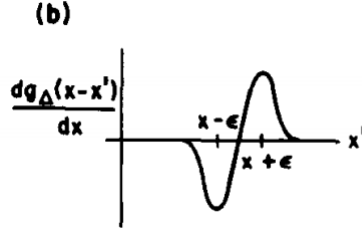
From Gaussian model, we know that the delta function is not only real but also even:

$$\delta(x - x') = \delta(x' - x). \tag{96}$$

Next, we consider the derivative of $\delta(x - x')$ with respect to x:

$$\delta'(x - x') = \frac{d}{dx}\delta(x - x'). \tag{97}$$

Once again, we consider the Gaussian model. We consider $dg_\Delta(x - x')/dx = -dg_\Delta(x - x')/dx'$ as a function of x':

(b)

1.13.2   Operators in Infinite Dimensions

19

2 Review of Classical Mechanics

3 All is Not Well with Classical Mechanics

4 The Postulates –a General Discussion

5   Simple Problems in One Dimension

6   The Classical Limit

7 The Harmonic Oscillator

8 The Path Integral Formulation of Quantum Theory

9 The Heisenberg Uncertainty Relation

10   Systems with N Degrees of Freedom

11 Symmetries and Their Consequences

12 Rotational Invariance and Angular Momentum

13   The Hydrogen Atom

14 Spin

15 Additional of Angular Momentum

16 Variational and WKB Methods

17   Time-Independent Perturbation Theory

18   Time-Dependent Perturbation Theory

19 Scattering Theory

20　The Dirac Equation

21   Path Integrals–II

22 Selected Problems and Solutions

22.1 Mathematical Introduction

22.2 Review of Classical Mechanics

22.3 All is Not Well with Classical Mechanics

22.4 The Postulates –a General Discussion

22.5 Simple Problems in One Dimension

22.6   The Classical Limit

22.7   The Harmonic Oscillator

22.8   The Path Integral Formulation of Quantum Theory

22.9   The Heisenberg Uncertainty Relation

22.10 Systems with N Degrees of Freedom

22.11   Symmetries and Their Consequences

22.12 Rotational Invariance and Angular Momentum

22.13   The Hydrogen Atom

22.14 Spin

22.15 Additional of Angular Momentum

22.16 Variational and WKB Methods

22.17   Time-Independent Perturbation Theory

22.18   Time-Dependent Perturbation Theory

22.19   Scattering Theory

22.20　The Dirac Equation

22.21   Path Integrals–II