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Part I

MATHEMATICAL TOOLS FOR QM

1

INTRODUCTION

The chief obstacle to the assimilation of the postulates of quantum mechaniics is not the postulates themselves, but rather the large body of linear algebraic notions required to understand them. Coupled with the unusual Dirac notations adopted by physicist in quantum mechanics, it can appear quite fearsome.

A good understanding of quantum mechanics is based upon a solid grasp of elementary linear algebra.

2

BRAC AND KET

Dirac Notation: elements, $|\psi\rangle$, of a Hilbert space is the physical state of a quantum system. This state can be specified through expaonsion using a basis vector. To free state vectors from coordinate meaning, Dirac introduced a notation in quantum mechanics, this makes the formalism of quantum mechanics with ease and clarity.

Three mathematical objects of QM:

1. Brac, $\langle\psi|$: elements of a Hilbert vector space
2. Ket, $|\psi\rangle$: elements of a dual space
3. Brac-ket, $\langle\phi|\psi\rangle$: Dirac notation for the scalar (inner) product

To obtain measureable quantities, we have to single out a particular representation basis

Position representation:

$$\begin{aligned} \langle r,t|\psi\rangle &= \psi(r,t) \\ \langle\phi|\psi\rangle &= \int \phi^*(r,t)\psi(r,t)d^3r \end{aligned} \tag{1}$$

Momentum representation:

$$\begin{aligned} \langle p,t|\psi\rangle &= \psi(p,t) \\ \langle\phi|\psi\rangle &= \int \phi^*(p,t)\psi(p,t)d^3p \end{aligned} \tag{2}$$

Properties of bra and ket.

1. Norm

$$|\langle\phi|\psi\rangle|^2 \text{ is defined to be the norm of } |phi\rangle, |psi\rangle$$

2. Orthogonality

$$\langle\phi|\psi\rangle = 0, \; |\phi\rangle \text{ and } \langle\psi| \text{ are said to be orthogonal}$$

3. Schwartz inequality

$$|\langle\phi|\psi\rangle|^2 \leq \langle\phi|\phi\rangle\langle\psi|\psi\rangle$$

4. Triangle inequality

$$\sqrt{\langle\phi+\psi|\phi+\psi\rangle} \leq \sqrt{\langle\psi|\psi\rangle} + \sqrt{\langle\phi|\phi\rangle}$$

5. Orthonormal

$$\langle\psi|\phi\rangle = 0, \text{ where } \langle\psi|\psi\rangle = 1 \text{ and } \langle\phi|\phi\rangle = 1$$

3

OPERATORS

Operator is a mathematical rule to transform a ket $|\psi\rangle$ into another ket $|\psi'\rangle$ of the same space.

$$\hat{A}|\psi\rangle = |\psi'\rangle$$

$$\langle r|\hat{A}|\psi\rangle$$

$$\langle\psi|\hat{A} = \langle\psi'|$$

Examples of Operators:

1. Unity Operator:

$$I\langle\psi| = \langle\psi|$$

2. Gradient Operator:

$$\nabla|\psi\rangle = \sum_i^3 \frac{\partial\psi}{\partial x_i}\hat{x}_i$$

3. Linear Momentum Operator:

$$\hat{P}\psi(r,t) = -i\hbar\nabla\psi(r,t)$$

4. Laplacian Operator:

$$\nabla^2\psi(r,t) = \sum_i^3 \frac{\partial^2\psi}{\partial {x_i}^2}\hat{x}_i$$

5. Parity Operator:

$$\mathcal{P}\psi(r) = \psi(-r)$$

3.1 PROPERTIES

Operators possesses special properties. Familiarizing it will be of great help in applications of operators in dirac notations. Here are some important properties one has to note on operators:

1. Product of Operators: the order of the application of operator is important. For the following operator, $\hat{A}$, $\hat{B}$, $\hat{C}$.

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

   However, they are associative.

$$\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$$

2. Linearity:

$$\hat{A}(a\,|\psi\rangle + b\,|\phi\rangle) = a\hat{A}\,|\psi\rangle + b\hat{A}\,|\phi\rangle$$

3. Expectation/Mean Values
4. Hermitean Adjoint
   a) Projectors: a subclass of Hermitean Adjoint

3.2 FUNCTIONS ON OPERATORS

3.3 COMMUTATOR ALGEBRA

In mathematicas, commutator gives an indication of the extent to which a certain binary operation fails to be commutative. There are different definitions used in group theory and ring theory. The one utilized in quantum mechanics is the definition of ring theory. In quantum mecahnics, commutation is not just a mathematical operation, it has an implication that allows one to simplify the identification of an eigenfunction [1].

Commutation between two operators $\hat{A}$ and $\hat{B}$, is defined by

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Anticommutator is define as,

$$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

if $[\hat{A}, \hat{B}] = 0$, $\hat{A}$ and $\hat{B}$ are said to commute, which means that $\hat{A}\hat{B} = \hat{B}\hat{A}$.

Hermitean operators always commute. To see these, assume $\hat{A}$ and $\hat{B}$ are hermitean, $\hat{A} = \hat{A}^\dagger$ and $\hat{B} = \hat{B}^\dagger$. Note also that Hermitean operator's product is also Hermitean.

$$\begin{aligned} (\hat{A}\hat{B})^\dagger &= \hat{B}^\dagger\hat{A}^\dagger \\ (\hat{A}\hat{B})^\dagger &= \hat{B}\hat{A} \\ (\hat{A}\hat{B})^\dagger &= \hat{A}\hat{B} \end{aligned} \tag{3}$$

Therefore, the hermitean operators $\hat{A}$ and $\hat{B}$ always commute, $\hat{A}\hat{B} = \hat{B}\hat{A}$.

For position representation of momentum, the following commutation relation are always satisfied.

$$\begin{aligned} [\hat{X}, \hat{P}_x] &= i\hbar I \\ [\hat{Y}, \hat{P}_y] &= i\hbar I \\ [\hat{Z}, \hat{P}_z] &= i\hbar I \end{aligned} \tag{4}$$

1 see chapter 10

The following properties are useful in solving commutation relations of some operators in Quantum mechanics, familiarizing them would be of great help in the future.

1. antisymmetry:

$$[\hat{A},\hat{B}] = -[\hat{B},\hat{A}] \tag{5}$$

2. linearity:

$$[\hat{A},\hat{B}+\hat{C}+\hat{D}] = [\hat{A},\hat{B}]+[\hat{A},\hat{C}]+[\hat{A},\hat{D}] \tag{6}$$

3. distributivity[2]:

$$\begin{aligned}[\hat{A},\hat{B}\hat{C}] &= [\hat{A},\hat{B}]\hat{C}+\hat{B}[\hat{A},\hat{C}]\\ [\hat{A}\hat{B},\hat{C}] &= [\hat{A},\hat{C}]\hat{B}+\hat{A}[\hat{B},\hat{C}]\end{aligned} \tag{7}$$

4. Operator commutation with scalars:

$$[\hat{A},b] = 0$$

5. jacobi identity[3]:

$$[\hat{A},[\hat{B},\hat{C}]]+[\hat{B},[\hat{C},\hat{A}]]+[\hat{C},[\hat{A},\hat{B}]] = 0 \tag{8}$$

6. repeated application of distributivity property:

$$\begin{aligned}[\hat{A},\hat{B}^n] &= \sum_{j=0}^{n-1}\hat{B}^j[A,B]\hat{B}^{n-j-1}\\ [\hat{A}^n,\hat{B}] &= \sum_{j=0}^{n-1}\hat{A}^{n-j-1}[A,B]\hat{A}^j\end{aligned} \tag{9}$$

7. hermitean conjugate of a commutation:

$$[\hat{A},\hat{B}]^\dagger = [\hat{B}^\dagger,\hat{A}^\dagger] \tag{10}$$

2 in other books this is referred to as the Leibniz Rules
3 useful in Lie Algebra to check the commutativity

4

MATRIX REPRESENTATION

Let $|\phi_n\rangle$ be a discrete, complete and orthonormal basis, the following properties are true: Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Ut purus elit, vestibulum ut, placerat ac, adipiscing vitae, felis. Curabitur dictum gravida mauris. Nam arcu libero, nonummy eget, consectetuer id, vulputate a, magna. Donec vehicula augue eu neque. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Mauris ut leo. Cras viverra metus rhoncus sem. Nulla et lectus vestibulum urna fringilla ultrices. Phasellus eu tellus sit amet tortor gravida placerat. Integer sapien est, iaculis in, pretium quis, viverra ac, nunc. Praesent eget sem vel leo ultrices bibendum. Aenean faucibus. Morbi dolor nulla, malesuada eu, pulvinar at, mollis ac, nulla. Curabitur auctor semper nulla. Donec varius orci eget risus. Duis nibh mi, congue eu, accumsan eleifend, sagittis quis, diam. Duis eget orci sit amet orci dignissim rutrum.

1. $\langle\phi_m|\phi_n\rangle = \delta_{mn}$

4.1 DISCRETE BASES

4.1.1 *Brac*

4.1.2 *Ket*

4.1.3 *Operators*

4.1.4 *Other Quantities*

4.2 CONTINUOUS BASES

4.2.1 *Brac*

4.2.2 *Ket*

4.2.3 *Operators*

4.2.4 *Other Quantities*

5

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Part III

APPENDIX

A

APPENDIX CHAPTER

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A.1 A SECTION

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