chmy564-17
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1. Separability in General

2. Dirac Notation :Symbolic vs shorthand
   Hilbert Space
   Vectors,

Theorems vs. Postulates

The 3 body problem is not solvable in classical or QM
Approximations, however, can be more accurate than experiment,
(given enough computer power and time)

Thus we soon will start learning/reviewing the Variation Principle and methods,
which are the foundation of computational quantum chemistry.

First: Briefly review underlying notations, theorems and postulates of QM Use Chapter 7 of Levine as guide--but interject quotations from Dirac;

First: Notation from Levine: $\int f_m^* \hat{A} f_n \, d\tau \equiv \left\langle f_m \middle| \hat{A} \middle| f_n \right\rangle \equiv \left\langle m \middle| \hat{A} \middle| n \right\rangle \equiv A_{mn}$

bracket notation “introduced by Dirac”
and later on p 166 Levine states: We will occasionally use a notation (called **ket** notation in which an arbitrary function *f* is dnoted by the symbol |*f*>. There doesn’t seem to be any point to this notation, but in advance formulations of QM, it takes on a special significance.

Whereas Levine mostly considers this just shorthand, clearly Dirac had a deeper meaning in mind:

Quotes from Dirac preface, 1930 ("Reading 1")

field. For this reason a book on the new physics, if not purely descriptive of experimental work, must be essentially mathematical. All the same the mathematics is only a tool and one should learn to hold the physical ideas in one's mind without reference to the mathematical form. In this book I have tried to keep the physics to the forefront,

presented, an author must decide at the outset between two methods. There is the symbolic method,* which deals directly in an abstract way with the quantities of fundamental importance (the invariants, etc., of the transformations) and there is the method of coordinates or representations, which deals with sets of numbers corresponding to these quantities. The second of these has usually been used for the

bra and ket

wavefunctions and matrices

The symbolic method, however, seems to go more deeply into the nature of things. It enables one to express the physical laws in a neat and concise way, and will probably be increasingly used in the future as it becomes better understood and its own special mathematics gets

Paraphrased from Dirac:

Superposition principle suggests states are infinite set of complex ***vectors***

which he named: ***kets* , |>**

Then noted “Whenever we have a set of vectors in any mathematical theory, we can always set up another set of vectors ... the dual vectors... , which he called **bra** vectors, <|, and which together make brackets.

We have the rules that ***any complete bracket expression denotes a number and any incomplete bracket expression denotes a vector of the bra or ket kind***.

We now make the assumption of one-to-one correspondence between the bras and kets, ... and the bra corresponding to c|A> is <A|c*

... any state of our dynamical system at a particular time may be specified by the direction of a bra vector just as well as by the direction of the ket..
...the whole theory will be symmetrical regarding bras and kets.

This was later recognized as a ***Hilbert space***

Lowdin later stated: "The mathematics of QM is that of **analytic geometry.**

Other notational statements by Levine $\langle m|n\rangle^* = \langle n|m\rangle$

$$\left\langle cf \left| \hat{B} \right| g \right\rangle = c^* \left\langle f \left| \hat{B} \right| g \right\rangle \text{ and } \left\langle f \left| \hat{B} \right| cg \right\rangle = c \left\langle f \left| \hat{B} \right| g \right\rangle$$

Next: 9 Theorems and 5 Postulates

theorem: can be proved by chain of reasoning; a truth established by accepted truths.

postulate: accepted as true without proof.

7.2 Hermitian operators

$$\int \Psi^* \hat{A} \Psi \; d\tau = \langle \mathrm{A} \rangle = \langle \mathrm{A} \rangle^* \text{ for real (physical) operators}$$

One definition of Hermitian often seen is: $\int \Psi^* \hat{A} \Psi \; d\tau = \left[\int \Psi^* \hat{A} \Psi \; d\tau \right]^* = \int \Psi \left(\hat{A} \Psi \right)^* d\tau$

An other, seemingly more powerful, is: $\int f^* \hat{A} g \; d\tau = \int g \left(\hat{A} f \right)^* d\tau$

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Theorem 1. The eigenvalues of an Hermitian operator are real numbers

Theorem 2. The eigenfunctions of an Hermitian operator are orthogonal—unless the eigenvalues are degenerate. They can be made orthogonal, however

Postulate 4. *If B is a linear Hermitian operator that represents a physical property, the eigenfunctions g_i of B form a complete set*

This must be a postulate because there are Hermitian operators whose eigenfunctions do not form compete set!