Commutators and Time Dependence *
(Dated: January 15, 2001)

I. REVIEW OF DIRAC NOTATION

The Dirac notation was invented to cut down on the amount of writing one does in actually "doing" quantum mechanics. This was a huge consideration in the "olden days" before computers, when typewriters had a fixed type face.

Conventionally, we write

$$H_{op}\psi = E\psi$$

as a statement of the Schrödinger Equation (time independent), i.e., the common eigenvalue problem. Once solved, the eigenstates are commonly labelled using some indicator of which particular eigenvalue is being addressed. Thus, one might write

$$H_{op}\psi_n = E_n\psi_n$$

for the n^{th} eigenstate associated with the n^{th} eigenvalue. In Dirac notation, this becomes

$$H_{op}|n >= E_n|n >$$

(or, possibly redundantly, $H_{op}|\psi_n >= E_n|\psi_n >$ where the economy of writing is obtained when the relevant indices inside the bra ($| >$) are all that are included, all others excluded. This compactness of notation means that lots of understanding has to be brought to the reading of these equations (by the way, we will often omit the 'op' subscript).

II. INTEGRALS IN DIRAC NOTATION

Consider two eigenfunctions ψ_n and ψ_m and the integral of some operator, O_{op} (for example, the dipole moment operator's important part, x_{op}), attempting something like the evaluation of a dipole selection rule, as an example. We would have

$$\int \psi_m^* O_{op}\psi_n d\tau = \int \psi_m^* \left(O_{op}\psi_n\right) d\tau$$

This integral is re-written as $< m|O_{op}|n >$ where $| >$ is the ket and $< |$ is the bra, and the two from a BRAcKET (Hah).

The left hand, bra, is understood to be the complex conjugate ($\imath \rightarrow -\imath$).

III. INTEGRALS, AN EXAMPLE

For the harmonic oscillator, as an example, the wave functions are known to be of the form

$$H_n(x)e^{-\alpha\frac{x^2}{2}}$$

with associated energy eigenvalues $\left(n+\frac{1}{2}\right)\hbar\omega$ In Dirac notation, this would be

$$\left(\frac{p^2}{2m} + k\frac{x^2}{2}\right)|n >= \left(n+\frac{1}{2}\right)\hbar\omega|n >$$

where the Hamiltonian is $\left(\frac{p^2}{2m} + k\frac{x^2}{2}\right)$. Writing $H|n >= E_n|n >$ is as compact as it gets.

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If asked for the expectation value of the x-coordinate (as an example), one would conventionally write

$$\int_{-\infty}^{\infty} H_n^*(x)e^{-\alpha\frac{x^2}{2}} x_{op} H_n(x)e^{-\alpha\frac{x^2}{2}} dx$$

(where $x_{op} = x$ and assuming that the complete wave functions $H_n(x)e^{-\alpha\frac{x^2}{2}}$ were normalized), as $< n|x|n >$ or as

$$\frac{< n|x|n >}{< n|n >}$$

if not-prenormalized.

This translates into, for n=zero,

$$\frac{\int_{-\infty}^{\infty} e^{-\alpha x^2/2} x e^{-\alpha x^2/2} dx}{\int_{-\infty}^{\infty} e^{-\alpha x^2/2} e^{-\alpha x^2/2} dx}$$

IV. THE TIME DEPENDENT SCHRÖDINGER EQUATION

The time dependent Schrödinger Equation is

$$\frac{d| >}{dt} = \frac{1}{\hbar\imath} H_{op}| >$$

and if H_{op} does not explicitly depend on time, then this equation is variable separable, and we have (in functional notation)

$$\Psi(x, y, z, t) = \psi(x, y, z)g(t)$$

where

$$\frac{\partial\Psi}{\partial t} = \frac{1}{\imath\hbar} H_{op}\Psi - \frac{\imath}{\hbar} H_{op}\Psi$$

which becomes

$$\psi(x, y, z)\frac{\partial g(t)}{\partial t} = g(t)\frac{1}{\imath\hbar} H_{op}\psi(x, y, z)$$

so $g(t) = e^{\kappa t}$ and

$$\frac{\partial g(t)}{\partial t} = \kappa g(t)$$

so that

$$\psi(x, y, z)\kappa g(t) = g(t)\frac{1}{\imath\hbar} H_{op}\psi(x, y, z)$$

and, since g(t) now cancels on both sides, we have the time independent Schrödinger Equation

$$\psi(x, y, z)\kappa = \frac{1}{\imath\hbar} H_{op}\psi(x, y, z) = -\frac{\imath}{\hbar} H_{op}\psi$$

Continuing, we have

$$H_{op}\psi(x, y, z) = -\frac{\imath}{\hbar}\kappa\psi(x, y, z)$$

and conventionally, we then have

$$-\frac{\hbar}{\imath}\kappa = E$$

i.e., $H_{op}\psi(x, y, z) = E\psi(x, y, z)$, and $\kappa = -\frac{E\imath}{\hbar}$ so the full time dependent wave function for eigenstates would be

$$\Psi(x, y, z, t) = e^{-\frac{\imath Et}{\hbar}}\psi(x, y, z)$$

V. SOME DEFINITIONS

1. An operator, O_{op} is linear if

$$O_{op}(c\psi) = cO_{op}\psi$$

and

$$O_{op}(\psi_1 + \psi_2) = cO_{op}(\psi_1 + \psi_2)$$

2. An operator is Hermitian if

$$\int (O_{op}\psi)^* \psi d\tau = \int \psi^* O_{op}\psi d\tau$$

i.e., $< O_{op}\psi|\psi >=< O_{op}\psi|\psi >^* =< \psi|O_{op}\psi >$ Further, $< \psi_1|O_{op}\psi_2 >=< O_{op}\psi_1|\psi_2 >$

3. A Hermitian operator is "self adjoint", i.e., Hermitian Adjoint if

$$< \psi_1|(O_{op}\psi_2 >=< (O^\dagger_{op}\psi_1|\psi_2 >$$

4. The Eigenvalues of a Hermitian operator are real. If $O_{op}\psi_n = q_n\psi_n$ and $O_{op} = O^\dagger_{op}$ (and assuming the eigenfunction to be normalized) we have $< n|O_{op}n >=< n|q_n n >= q_n < n|n >= q_n$ and $< O_{op}n|n >=< q_n n|n >= q_n^* < n|n >= q_n^*$ But these two are equal, hence $q_n^* = q_n$.

5. The eignefunctions of a Hermitian operator are orthogonal if they correspond to different eigenvalues. If $O_{op}\psi_1 = q_1\psi_1$ and $O_{op}\psi_2 = q_2\psi_2$ then $< 1|O_{op}2 >= q_2 < 1|2 >$ and $< O_{op}1|2 >= q_1 < 1|2 >$ so subtracting, we have $0 = (q_2 - q_1 i) < 1|2 >$ and if the eigenvalues are distinct, then the integral must be zero.

6. the expectation value of an operator is

$$< q >= \frac{\int \psi O_{op}\psi d\tau}{\int \psi\psi d\tau}$$

VI. EXPECTATION VALUES

We need to look at the time dependence of the expectation value of some operator (observable) such as "x", i.e., what is

$$\frac{d < |x| >}{dt} = \frac{d \int \psi^* x\psi d\tau}{dt}$$

assuming that we are in a state $\psi(x, t)$. Then we have (using a mixed notation)

$$\frac{d < |x| >}{dt} = \frac{d \int \psi^* |x| \psi d\tau}{dt} = \int \left(\frac{d\psi^*}{dt} x\psi + \psi^* \frac{dx}{dt}\psi + \psi^* x \frac{d\psi}{dt} \right) d\tau$$

where the explicit time dependence of the operator x on t is included in the middle term. But the time dependent Schrödinger Equation is

$$\frac{d| >}{dt} = \frac{1}{\imath\hbar} H_{op}| >$$

and

$$\frac{d < |}{dt} = -\frac{1}{\imath\hbar} H^*_{op} < |$$

or (in more conventional notation)

$$\frac{\partial\psi}{\partial t} = \frac{1}{\imath\hbar} H_{op}\psi$$

and

$$\frac{\partial \psi^*}{\partial t} = -\frac{1}{\imath\hbar}(H_{op}\psi)^*$$

so, assuming the x-operator is not an explicit function of time (so the middle term vanishes, we have

$$\frac{d < x >}{dt} = -\frac{1}{\imath\hbar} < |H_{op}x| > + \frac{1}{\imath\hbar} < |xH_{op}| >$$

where $\int (H\psi)^* x\psi = \int \psi^* Hx\psi$ which is true for all Hermitian operators. which yields

$$\frac{d < |x| >}{dt} = +\frac{1}{\imath\hbar} < | \, (H_{op}x - xH_{op}) \, | >$$

Since

$$\frac{d < |x| >}{dt} = \frac{1}{\imath\hbar} < [H_{op}, x] >$$

if the commutator is zero, then the change in the average value with time is also zero which implies that the average value is a constant in time.

What does this mean? It means that that time derivative of something is zero, which means that when integrating, one obtains that the $< |x| >$ value is constant in time. In classical mechanics, something that is constant in time is called a constant of the motion. Such things have a special place of importance in classical mechanics. They also have a special place (of honor) in quantum mechanics.

The commutator is central to the discussion of simultaneous measurements. Consider a state which is a simultaneous eigenfunction of two operators. The means the $A_{op}| >= \alpha| >$ and $B_{op}| >= \beta| >$ then

$$A_{op} \left[B_{op}| > \right] = A_{op}\beta| >= \beta A_{op}| >$$

and this means that the eigenfunction of B_{op} is also an eigenfunction of A_{op}. Furthermore,

$$B_{op} \left[A_{op}| > \right] = B_{op}\alpha| >= \alpha B_{op}| >$$

so, subtracting, we have

$$A_{op} \left\{ B_{op}| > \right\} - B_{op} \left\{ A_{op}| > \right\} = \beta A_{op}| > -\alpha B_{op}| >= \beta\alpha| > -\alpha\beta| >= 0$$

Thus, if a function is a simultaneous eigenfunction of two variables, then the operators commute and *vice versa*.

VII. MORE COMMENTS ABOUT HERMITIAN OPERATORS

To each physical observable is associated a linear, Hermitian operator. Eigenvalues of this operator are the only values of this observable which can be obtained by direct measurement.

An operator is linear if

$$Q_{op}(c\psi) = cQ_{op}(\psi)$$

and

$$Q_{op}(\psi_1 + \psi_2) = Q_{op}\psi_1 + Q_{op}\psi_2$$

An operator is Hermitian if

$$\int (Q_{op}\psi)^* \psi d\tau = \int \psi^* Q_{op}\psi d\tau$$

where $d\tau$ is the appropriate differential volume element. In Dirac notation this would be

$$< Q_{op}\psi|\psi >=< Q_{op}\psi|\psi >^* =< \psi|Q_{op}\psi >$$

A Hermitian operator is self-adjoint. If

$$< \psi_1|Q_{op}\psi_2 >=< Q_{op}^\dagger \psi_1|\psi_2 >$$

i.e., if the Hermitian adjoint, $Q_{op}^\dagger$, of the operator Q_{op}, obeys the relation: $Q_{op} = Q_{op}^\dagger$ then Q_{op} is Hermitian. Under those circumstances, for Hermitian operators one can write $< \psi_1|Q_{op}|\psi_2 >$ where Q_{op} operates either right or left, i.e., operates on ψ_1 or on ψ_2.