

# THE INTERACTION OF RADIATION AND MATTER: SEMICLASSICAL THEORY

## I. REVIEW OF BASIC QUANTUM MECHANICS: CONCEPTS, POSTULATES AND NOTATION:

At the outset, let us, briefly, reconsider why quantum mechanics is necessary?

- Forces known in classical electrodynamics cannot account for the remarkable stability of atoms and molecules.
- Disturbed dynamic systems radiate only frequencies which may be expressed as differences between certain values (Ritz's Combination Law of Spectroscopy).<sup>1</sup>
- All physical systems -- *viz.* material "particles" and electromagnetic fields -- exhibit *wave-particle duality* -- *i.e.* to explain particular observations the system must in some instances be modeled as a particle and in others as a wave.
- There is a limit below which the disturbance associated with a observation is not negligible and, thus, there is an unavoidable *indeterminacy* in the prediction of observed results.

To proceed, we recall an ancient comment of P. A. M. Dirac:<sup>2</sup>

"Quantum mechanics...requires the states of a dynamic system and the dynamical variables to be to be interconnected in quite strange ways that are unintelligible from the classical standpoint. The states and dynamic variables have to be represented by mathematical quantities of different natures from those ordinarily used in physics"

Following the Master we begin with the general quantum mechanical *principle of superposition of states*. To quote him once more:

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<sup>1</sup> According to classical theory, a disturbed system should radiate certain fundamental frequencies and their harmonics. Each fundamental frequency would be associated with one of the systems degrees of freedom.

<sup>2</sup> P. A. M. Dirac, *The Principles of Quantum Mechanics* (Revised fourth edition), Oxford University Press (1967).

"The non-classical nature of the superposition process is brought out clearly if we consider the superposition of two states, A and B, such that there exists an observation which, when made on the system in state A, is certain to lead to one particular result, **a** say, and when made on the system in state B is certain to lead to some different result, **b** say. What will be the result of the observation when made on the system in the superposed state? The answer is that the result will be sometimes **a** and sometimes **b**, according to a probability law depending on the relative weights of A and B in the superposition process. It will never be different from both **a** and **b**. *The intermediate character of the state formed by superposition thus expresses itself through the probability of a particular result for an observation being intermediate between the corresponding probabilities for the original states, not through the result itself being intermediate between the corresponding results for the original states.*

"...The superposition process is a kind of additive process and implies that states can in some way be added to give new states. The states must therefore be connected with mathematical quantities of a kind which can be added together to give other quantities of the same kind. The most obvious of such quantities are vectors"

With this motivation, Dirac introduced the whimsical name *ket* and the ingenious right half-bracket notation --  $| \rangle$  -- to represent the vectors connected to the states of a quantum mechanical system.<sup>3</sup> Thus, the superposition of two states to form a third is represented in abstract ket vector notation, as

$$|R\rangle = c_1 |A\rangle + c_2 |B\rangle \quad [ I-1a ]$$

where the  $c_n$ 's may be complex numbers. More generally,

<sup>3</sup> The state is specified by **the direction** of a ket vector and any length assigned to the vector is irrelevant.

$$|R\rangle = c| \rangle + c' | \rangle \quad [ I-1b ]$$

For any set of vectors one can always define a complementary set of dual vectors. In Dirac's development, the dual vectors are called **bra** vectors and denoted by the other half of the *bracket* symbol  $\langle \rangle$ . A bra vector  $\langle P|$  is completely defined when its scalar product -- i.e.  $\langle P||Q\rangle = \langle P|Q\rangle$  -- with every ket vector  $|Q\rangle$  is known. The scalar product is linear (or anti-linear) in the sense that:

$$\langle B| \{ |A\rangle + |A\rangle \} = \langle B|A\rangle + \langle B|A\rangle \quad [ I-2a ]$$

$$\langle B| \{ c|A\rangle \} = c\langle B|A\rangle \quad [ I-2b ]$$

$$\{ \langle B| + \langle B| \} |A\rangle = \langle B|A\rangle + \langle B|A\rangle \quad [ I-2c ]$$

$$\{ c\langle B| \} |A\rangle = c\langle B|A\rangle \quad [ I-2d ]$$

$$\text{If } \langle P|A\rangle = 0 \text{ for all } |A\rangle, \text{ then } \langle P| = 0. \quad [ I-2e ]$$

Although bras and kets are very different creatures, **it is assumed** that there is a one-to-one correspondence between bras and kets such that the bra corresponding to the ket  $|A\rangle + |A\rangle$  is the sum of the bras corresponding to the kets  $|A\rangle$  and  $|A\rangle$  -- viz.  $\langle A| + \langle A|$  -- and the bra corresponding to the ket  $c|A\rangle$  is the product of  $c$  times the bra corresponding to the ket  $|A\rangle$  -- viz.  $c\langle A|$ .<sup>4</sup> It is also assumed (**an especially**

<sup>4</sup> Dirac uses the words **conjugate imaginary** to connote a corresponding bra-ket pair and, thereby, draws attention to an important distinction. The words **conjugate complex** are reserved for the pairing of ordinary complex quantities which can be split into real and imaginary parts. In particular, the real part of a complex quantity is given by one half of the sum of the quantity and its conjugate complex. However, bras and kets are representations in dual vector spaces and cannot be added!

**important assumption**) that  $\langle P|Q\rangle = \langle Q|P\rangle$  -- so that  $\langle P|P\rangle$  is real -- and that  $\langle P|P\rangle \geq 0$ .<sup>5</sup>

To briefly recapitulate, the directions of vectors of a dual abstract vector space are to be associated with states of a dynamic system. To extend the Diracian view, dynamic variables and observables of the system are to be associated with (real) abstract **linear operators** which transform one vector into an other -- *viz.*

$$|F\rangle = Op |A\rangle . \quad [ I-3 ]$$

Linearity requires that  $Op\{|A\rangle + |A'\rangle\} = Op |A\rangle + Op |A'\rangle$  [ I-4a ]

and  $Op\{c |A\rangle\} = c Op |A\rangle$  [ I-4b ]

The conjugate imaginary or adjoint of  $|F\rangle$  is obtained by operating (to the left) with the **hadjoint** of the linear operator <sup>6</sup> on the conjugate imaginary of  $|A\rangle$  -- *viz.*

$$\langle F| = (|F\rangle)^\dagger = (Op |A\rangle)^\dagger = \langle A| Op^\dagger . \quad [ I-5 ]$$

By assumption  $\langle P|Q\rangle = \langle Q|P\rangle$  so that

$$\langle A| Op^\dagger |F\rangle = \langle F| Op |A\rangle \quad [ I-6 ]$$

From which we may easily show that

$$Op^{\dagger\dagger} = Op \quad [ I-7a ]$$

<sup>5</sup> We may thus identify the numbers  $\langle P|Q\rangle$  as elements of a hermitian matrix -- Charles Hermite (1822-1901).

<sup>6</sup> If a linear operator corresponds to a dynamic variable, then the adjoint of that operator corresponds to the conjugate complex of the dynamic variable.

and 
$$(Op_1 Op_2)^\dagger = Op_2^\dagger Op_1^\dagger \quad [ I-7b ]$$

To further develop the notion of linear operators, we examine the *eigenvalue* equation

$$\mathcal{A} |F\rangle = a |F\rangle \quad [ I-8 ]$$

where  $\mathcal{A}$  is a linear operator and  $a$  is a number. In most instances, the equation arises in a context wherein  $\mathcal{A}$  is a known linear operator, which corresponds to a dynamic variable, and the number  $a$  -- an eigenvalue -- and the ket  $|F\rangle$  -- an eigenvector -- are unknowns to be determined. Only self-adjoint (*i.e.* real or Hermitian) linear operators are of any use quantum mechanics so we may write quite generally

$$\mathcal{A} |P\rangle = p |P\rangle \quad [ I-9a ]$$

$$\langle Q| \mathcal{A} = q \langle Q| \quad [ I-9b ]$$

It follows that all eigenvalues are real numbers, that eigenvalues associated with eigenkets are the same as those associated with eigenbras, and that conjugate imaginary of any eigenket is an eigenbra belonging to the same eigenvalue (and conversely). If we may assume that a complete set of eigenvalues and eigenvectors of a given dynamic variable is known, we may use the following exquisitely self-explanatory notation to delineate the manifold of all eigenvalue equations:

$$| \rangle = | \rangle; | \rangle = | \rangle; | \rangle = | \rangle; \dots \dots \quad [ I-10 ]$$

It is easy to show that **within this manifold, the eigenvectors belonging to different eigenvalues are orthogonal!**

## REPRESENTATIONS AND QUANTUM CONDITIONS:

### GENERAL NOTIONS:

As pointed out earlier, a bra vector is completely defined in terms of a set of numbers -- the *representatives* -- which are the values of the scalar product of the bra with every ket in a *representation* (and conversely). Thus, if we have a complete set of discrete, orthonormal state vectors  $| \rangle$  we may write a superposition of discrete states as

$$| \rangle = \sum | \rangle \langle | \rangle \quad [ I-11a ]$$

If we have a complete set of continuous, orthonormal state ket vectors  $| \rangle$  we may write a superposition of continuous states as

$$| \rangle = \int d | \rangle \langle | \rangle \quad [ I-11b ]$$

Consideration of these two expansions leads to extremely valuable expressions for expansions of the **identity operator** -- viz.

$$I = \sum | \rangle \langle | \rangle \quad [ I-12a ]$$

or

$$I = \int d | \rangle \langle | \rangle \quad [ I-12b ]$$

This is, essentially, a diagonal **dyadic** representation of the identity operator. More generally, a linear operator has the following dyadic representation

$$Op = \sum | \rangle \langle | \langle | Op | \rangle \quad [ I-13a ]$$

or

$$Op = \sum | \rangle \langle | \langle | Op | \rangle d d \quad [ I-13b ]$$

Since commuting linear operators have simultaneous eigenstates, it is a critical matter to know whether or not two observables commute and, if they do not, to know the *commutation relation* needed to replace the classical *commutative law of multiplication*. Fortunately, the so called method of **classical analogy** provides a systematic means for establishing such relationships for the very large class of dynamic systems which obey the Euler-Lagrange equations of motion.<sup>7</sup> If such a system has  $n$  degrees of freedom, it is describable in terms of  $n$  pairs of **canonically conjugate** coordinates  $q_r$  and momenta  $p_r$ .<sup>8</sup> The essence of the method of classical analogy is embedded in statement that the **commutator is the quantum mechanical equivalent of the classical Poisson Bracket** and is given by

$$[u, v] = uv - vu = i\hbar \{u, v\}_{\text{PB}} = i\hbar \left( \frac{u}{q_r} \frac{v}{p_r} - \frac{u}{p_r} \frac{v}{q_r} \right) . \quad [\text{I-14}]$$

Thus, the **fundamental quantum conditions** or **commutation relationships** are

$$[q_r, q_s] = q_r q_s - q_s q_r = 0 \quad [\text{I-15a}]$$

<sup>7</sup> This class includes fields, in particular the electromagnetic field, as well as the mechanics of particle motion.

<sup>8</sup> Precisely: A pair of dynamic variables  $r$  and  $s$  are said to be canonically conjugate if there is function of the two variables  $\mathcal{H}(r, s)$  such that

$$\frac{dr}{dt} = \frac{\mathcal{H}}{s} \quad \text{and} \quad \frac{ds}{dt} = -\frac{\mathcal{H}}{r} .$$

For a second function of the canonical variables  $\mathcal{F}(r, s)$  we have

$$\frac{d\mathcal{F}}{dt} = \frac{\mathcal{F}}{r} \frac{dr}{dt} + \frac{\mathcal{F}}{s} \frac{ds}{dt} = \frac{\mathcal{F}}{r} \frac{\mathcal{H}}{s} - \frac{\mathcal{F}}{s} \frac{\mathcal{H}}{r} = \{ \mathcal{F}, \mathcal{H} \}_{\text{PB}}$$

where  $\{ \mathcal{A}, \mathcal{B} \}_{\text{PB}}$  is the classical **Poisson Bracket**.

$$[p_r, p_s] = p_r p_s - p_s p_r = 0 \quad [I-15b]$$

$$[q_r, p_s] = q_r p_s - p_s q_r = i\hbar \{q_r, p_s\}_{PB} = i\hbar \delta_{rs} \quad [I-15c]$$

These relationships provide the foundation for the analogy between quantum and classical mechanics and they show that classical mechanics may be regarded as the limiting case of quantum mechanics when  $\hbar$  tends to zero.

#### THE SCHRÖDINGER OR COORDINATE REPRESENTATION:

The canonical coordinate(s) is (are) diagonal in the Schrödinger representation so that

$$q_1 q_2 q_3 \cdots |q_1 q_2 q_3 \cdots\rangle = q_1 q_2 q_3 \cdots |q_1 q_2 q_3 \cdots\rangle \quad [I-16]$$

For simplicity, consider a system with a single degree of freedom. For such system any ket  $|q\rangle$  has a representative  $\langle q|q\rangle = 1$  -- *i.e.*

$$\langle q|q\rangle = \int dq |q\rangle \langle q|q\rangle = \int dq |q\rangle \langle q| \quad [I-17]$$

The linear operator  $d/dq$  acting on this ket generates a new ket which has a representative which is the derivative of the first representative -- *i.e.*

$$\frac{d}{dq} |q\rangle = \left| \frac{d}{dq} \langle q| \right| \quad [I-18a]$$

which means that

$$\left| \frac{d}{dq} (q) \right\rangle = dq |q\rangle \left\langle q \left| \frac{d}{dq} (q) \right\rangle = dq |q\rangle \frac{d}{dq} (q) .^9 \quad [ I-18b ]$$

Now the crucial commutator of  $q$  and  $d/dq$  may be obtain by the following argument:

$$\begin{aligned} \frac{d}{dq} q | (q) \rangle &= \frac{d}{dq} |q (q) \rangle = \left| \frac{dq}{dq} (q) \right\rangle = \left| q \frac{d}{dq} (q) \right\rangle + | (q) \rangle \\ &= q \frac{d}{dq} | (q) \rangle + | (q) \rangle \end{aligned} \quad [ I-19a ]$$

and, since  $| (q) \rangle$  is arbitrary,  $\frac{d}{dq} q - q \frac{d}{dq} = 1 . \quad [ I-19b ]$

Therefore, to be consistent with Equation [ I-15c ] we take

$$p_r = -i\hbar \frac{d}{dq} \dots \quad [ I-20 ]$$

THE MOMENTUM REPRESENTATION:

The canonical momenta are diagonal in the momentum representation<sup>10</sup> so that

$$p_1 p_2 p_3 \dots \dots \dots | p_1 p_2 p_3 \dots \dots \dots \rangle = p_1 p_2 p_3 \dots \dots \dots | p_1 p_2 p_3 \dots \dots \dots \rangle . \quad [ I-21 ]$$

By using Equations [ I-18b ] and [ I-20 ], we can show, for one degree of freedom, that the representative of the momentum in the Schrödinger representation is given by

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<sup>9</sup> It is easily shown that  $\left\langle (q) \left| \frac{d}{dq} = - \left\langle \frac{d}{dq} (q) \right| \right.$  which means that  $\frac{d}{dq}^\dagger = - \frac{d}{dq}$  and that  $\frac{d}{dq}$  is *apurely imaginary linear operator*.

<sup>10</sup> The momentum representation is, generally, less useful than the Schrödinger representation. Because of the manifest symmetry between  $q$  and  $p$  we can now easily show that  $q_r = i\hbar d/dp_r .$

$$\langle q | p | p \rangle = p \langle q | p \rangle = -i\hbar \langle q | \frac{\partial}{\partial q} | p \rangle = -i\hbar \frac{\partial}{\partial q} \langle q | p \rangle \quad [ I-22 ]$$

which has the solution  $\langle q | p \rangle = c(p) \exp(i p q / \hbar)$ . [ I-23 ]

This connection between the Schrödinger and momentum representations leads to the important insight: the coordinate (or momentum) representative of some arbitrary ket  $|A\rangle$  is given by the Fourier components of the momentum (or coordinate) representative -- *i.e.*

$$\langle p | A \rangle = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} \exp(-i p q / \hbar) dq \langle q | A \rangle \quad [ I-24a ]$$

$$\langle q | A \rangle = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} \exp(i p q / \hbar) dp \langle p | A \rangle \quad [ I-24b ]$$

Application of this transform pair to a *wave packets* in the Schrödinger representation leads directly to the Heisenberg Uncertainty Principle.

**A NOTE ON UNITARY TRANSFORMATIONS**

Let  $\mathcal{U}$  be any linear operator that has a reciprocal  $\mathcal{U}^{-1}$ . Consider the transformation

$$\mathcal{U}^\dagger = \mathcal{U} \mathcal{U}^{-1} \quad [ I-25 ]$$

where  $\mathcal{U}$  is an arbitrary linear operator. This may be interpreted as expressing a transformation from any linear operator  $\mathcal{U}$  to a corresponding operator  $\mathcal{U}^\dagger$ . The following properties hold:

- a.  $\mathcal{U}^\dagger$  has the same eigenvalues as the corresponding  $\mathcal{U}$  -- *i.e.* if  $\mathcal{U} | \psi \rangle = \lambda | \psi \rangle$  then

$$\mathcal{U} | \psi \rangle = \lambda | \psi \rangle \implies \mathcal{U}^{-1} \mathcal{U} | \psi \rangle = \mathcal{U}^{-1} \lambda | \psi \rangle = \lambda \mathcal{U}^{-1} | \psi \rangle \implies \mathcal{U}^\dagger \mathcal{U}^{-1} | \psi \rangle = \lambda \mathcal{U}^{-1} | \psi \rangle \quad [ I-26a ]$$

- b. The fundamental algebraic processes of addition and multiplication are left invariant by the transformation -- *e.g.*,

$$\begin{aligned} (U_1 + U_2)^T &= U (U_1 + U_2) U^{-1} = U U_1 U^{-1} + U U_2 U^{-1} = U_1^T + U_2^T \\ (U_1 U_2)^T &= U U_1 U_2 U^{-1} = U U_1 U^{-1} U U_2 U^{-1} = U_1^T U_2^T \end{aligned} \quad [ I-26b ]$$

- c. If  $U$  transforms a real  $U$  into a real  $U^T$

then  $U^T U = U$        $U^* U^T = U^*$

and  $U^* U^T U = U^* U$        $U^* U^T U = U^* U$

therefore  $U^* U = I$        $U^* = U^{-1}$       [ I-26c ]

Such a transformation is say to be a *unitary transformation*.