

THE INTERACTION OF RADIATION AND MATTER: QUANTUM THEORY

I. QUANTUM MECHANICS OF HARMONIC OSCILLATORS:¹

To prepare the ground for the quantization of the electromagnetic field, let us revisit the classical treatment of a simple harmonic oscillator with one degree of freedom. We start, with the assertion that the Hamiltonian of such an oscillator must have the form.

$$\mathcal{H} = \frac{1}{2m} [p^2 + m^2 \omega^2 q^2]. \quad [\text{I-1}]$$

where p and q are the canonically conjugate variables. Consequently, the accordant Hamilton equations yield a pair of coupled, inhomogeneous, first-order equations -- *viz.*

$$\frac{dq}{dt} = \frac{\mathcal{H}}{p} = p/m \quad [\text{I-2a}]$$

$$\frac{dp}{dt} = -\frac{\mathcal{H}}{q} = -m \omega^2 q. \quad [\text{I-2b}]$$

Combining these two equations, we see that formal classical analysis of the harmonic oscillator leads to a second-order homogeneous equation of motion

$$\frac{d^2q}{dt^2} = -\omega^2 q^2 \quad [\text{I-2c}]$$

with the evident complete solution

$$\begin{aligned} q(t) &= q(0) \cos \omega t + \frac{p(0)}{m} \sin \omega t \\ p(t) &= -m \omega q(0) \sin \omega t + p(0) \cos \omega t \end{aligned} \quad [\text{I-3}]$$

¹ William Louisell's *Radiation and Noise in Quantum Electronics*, McGraw-Hill (1964) has an excellent set of pre-quantum optics reviews.

Equations [I-2a] and [I-2b] are **decoupled** by transforming to a new set of dynamic variables -- viz.²

$$\begin{aligned} a &= \sqrt{\frac{m}{2}} [q + i p/m] \\ a^\dagger &= \sqrt{\frac{m}{2}} [q - i p/m] \end{aligned} \quad [I-4]$$

so that

$$\begin{aligned} q &= \frac{1}{\sqrt{2m}} [a + a^\dagger] \\ p &= i \sqrt{\frac{m}{2}} [a^\dagger - a] \end{aligned} \quad [I-5]$$

In terms of these new variables the Hamiltonian becomes

$$\mathcal{H} = a^\dagger a \quad [I-6]$$

Thus, Equations [I-2a] and [I-2b] are transformed to the decoupled **normal mode** form -- i.e.

$$\begin{aligned} \frac{da}{dt} &= -i a & i \frac{da}{dt} &= \frac{\mathcal{H}}{a^\dagger} = -i a \\ \frac{da^\dagger}{dt} &= i a^\dagger & i \frac{da^\dagger}{dt} &= -\frac{\mathcal{H}}{a} = i a^\dagger \end{aligned} \quad [I-7]$$

With this background, let us now turn to the quantum treatment of the harmonic oscillator. From the general theory discussed earlier, we make use of the **classical analogy** and postulate that the dynamic variables q and p become the Hermitian operators q and p which satisfy the commutation relations

² In classical theory, the a and a^\dagger variables are frequently referred to as normal mode amplitudes.

$$\begin{aligned} [q, q] &= 0 \\ [p, p] &= 0 \\ [q, p] &= i\hbar \end{aligned} \quad [I-8]$$

The Schrödinger representation of the energy eigenvectors -- *i.e.* $u_n(q) \langle q|E_n\rangle$ -- satisfies the following representations of the energy eigenvalue equation

$$\langle q | \mathcal{H} | E_n \rangle = E_n \langle q | E_n \rangle \quad [I-9a]$$

$$\langle q | \frac{1}{2m} [p^2 + m^2 q^2] | E_n \rangle = E_n \langle q | E_n \rangle \quad [I-9b]$$

$$\frac{1}{2m} \left[-\hbar^2 \frac{d^2}{dq^2} + m^2 q^2 \right] u_n(q) = E_n u_n(q) \quad [I-9c]$$

The solution to this equation is familiar as

$$u_n(q) = \sqrt{\frac{1}{2^n n!}} \sqrt{\frac{m}{\hbar}} H_n \left(\sqrt{\frac{m}{\hbar}} q \right) \exp \left[-\frac{m}{2\hbar} q^2 \right] \quad [I-10a]$$

where $H_n \left(\sqrt{\frac{m}{\hbar}} q \right)$ is one of the Hermite polynomials discussed in the set of lecture notes entitled *On Classical Electromagnetic Fields* and the corresponding eigenvalues are given by

$$E_n = \hbar \omega \left(n + \frac{1}{2} \right) \quad [I-10b]$$

An alternative treatment of the harmonic oscillator provides a powerful set of new tools. Recall the transformation law between state vectors in the Schrödinger and Heisenberg pictures -- *viz.*

$$|s(t)\rangle = \mathcal{T}(t,0) |s(0)\rangle = \exp\left[-\frac{i\mathcal{H}t}{\hbar}\right] |s(0)\rangle \quad [I-11]$$

which means that the operators transform according to the rules

$$\begin{aligned} q_H(t) &= \mathcal{T}^\dagger(t,0) q_S \mathcal{T}(t,0) \\ p_H(t) &= \mathcal{T}^\dagger(t,0) p_S \mathcal{T}(t,0) \end{aligned} \quad [I-12]$$

The Heisenberg equations of motion for q_H and p_H are

$$\frac{dq_H}{dt} = \frac{\mathcal{H}_H}{p_H} = p_H/m \quad [I-13a]$$

$$\frac{dp_H}{dt} = -\frac{\mathcal{H}_H}{q_H} = -m \omega^2 q_H \quad [I-13b]$$

By analogy with Equation [I-3], we see that the time evolution

$$\begin{aligned} q_H(t) &= \mathcal{T}^\dagger(t,0) q_S \mathcal{T}(t,0) = q_S \cos \omega t + \frac{p_S}{m} \sin \omega t \\ p_H(t) &= \mathcal{T}^\dagger(t,0) p_S \mathcal{T}(t,0) = -m \omega q_S \sin \omega t + p_S \cos \omega t \end{aligned} \quad [I-14]$$

is consistent with Equations [I-13a] and [I-13b]. By analogy with Equation [I-4] we introduce two critically important (non-Hermitian) operators -- *i.e.*

$$\begin{aligned} a &= \sqrt{\frac{m}{2\hbar}} \left[q + i p/m \right] \\ a^\dagger &= \sqrt{\frac{m}{2\hbar}} \left[q - i p/m \right] \end{aligned} \quad [I-15]$$

or

$$q = \sqrt{\frac{\hbar}{2m}} a + a^\dagger$$

$$p = i\sqrt{\frac{m\hbar}{2}} a^\dagger - a$$
[I-16]

with the commutation relation $[a, a^\dagger] = 1$ [I-17]

Thus

$$\mathcal{H} = \frac{\hbar}{2} [aa^\dagger + a^\dagger a] = \hbar [a^\dagger a + 1/2] = \hbar [\mathcal{N} + 1/2]$$
[I-18]

where $\mathcal{N} = a^\dagger a$ is an important (as yet uninterpreted) Hermitian operator (observable).
The Heisenberg equations of motion become

$$\frac{d\mathbf{a}_H}{dt} = \frac{1}{i\hbar} [\mathbf{a}_H, \mathcal{H}_H] = -i \mathbf{a}_H$$

$$\frac{d\mathbf{a}_H^\dagger}{dt} = \frac{1}{i\hbar} [\mathbf{a}_H^\dagger, \mathcal{H}_H] = +i \mathbf{a}_H^\dagger$$
[I-19]

with the solutions

$$a_H(t) = \mathcal{T}^\dagger(t,0) a_S \mathcal{T}(t,0) = a_S \exp(-i \omega t)$$

$$a_H^\dagger(t) = \mathcal{T}^\dagger(t,0) a_S^\dagger \mathcal{T}(t,0) = a_S^\dagger \exp(+i \omega t)$$
[I-20]

Consider the following equivalent eigenvalues problems -- viz.³

$$\mathcal{H} |E\rangle = E |E\rangle \quad \text{and} \quad \mathcal{N} |n\rangle = n |n\rangle$$
[I-21]

First note that

³ It follows from Equation [I-18] that $E = \hbar [n + 1/2]$.

$$\begin{aligned}
 [\mathcal{N}, a] &= \mathcal{N} a - a \mathcal{N} = a^\dagger a a - a a^\dagger a = [a^\dagger, a] a = -a \\
 [\mathcal{N}, a^\dagger] &= \mathcal{N} a^\dagger - a^\dagger \mathcal{N} = a^\dagger a a^\dagger - a^\dagger a^\dagger a = a^\dagger [a, a^\dagger] = a^\dagger
 \end{aligned}
 \tag{I-22a}$$

or

$$\begin{aligned}
 \mathcal{N} a &= a (\mathcal{N} - 1) \\
 \mathcal{N} a^\dagger &= a^\dagger (\mathcal{N} + 1)
 \end{aligned}
 \tag{I-22b}$$

Thus, we see that

$$\begin{aligned}
 \mathcal{N} \{a |n\rangle\} &= a (\mathcal{N} - 1)|n\rangle = (n - 1) a |n\rangle = (n - 1) |n - 1\rangle \\
 \mathcal{N} \{a^\dagger |n\rangle\} &= a^\dagger (\mathcal{N} + 1)|n\rangle = (n + 1) a^\dagger |n\rangle = (n + 1) |n + 1\rangle.
 \end{aligned}
 \tag{I-23}$$

That is, if $|n\rangle$ is an eigenket of the operator \mathcal{N} with eigenvalue n , then $a |n\rangle$ is also an eigenket, but with the eigenvalue $n - 1$. Similarly, if $|n\rangle$ is an eigenket of the operator \mathcal{N} with eigenvalue n , then $a^\dagger |n\rangle$ is an eigenvector with eigenvalue $(n + 1)$. Hence, the operators a and a^\dagger "generate" new eigenkets which have associated eigenvalues differing by one from eigenvalues associated with the original eigenkets. It follows that each eigenvalue of \mathcal{N} differs from all other eigenvalues by an integer!

Normalization of these eigenkets proceeds as follows:

Suppose

$$a |n\rangle = c_n |n - 1\rangle
 \tag{I-24}$$

Then

$$\begin{aligned}
 n \langle n | n \rangle &= \langle n | \mathcal{N} | n \rangle = \langle n | a^\dagger a | n \rangle = c_n \langle n | a^\dagger | n - 1 \rangle \\
 &= c_n \langle n - 1 | a | n \rangle = |c_n|^2 \langle n - 1 | n - 1 \rangle
 \end{aligned}
 \tag{I-25}$$

but we require $\langle n|n\rangle = \langle n-1|n-1\rangle = 1$ so that $c_n = \sqrt{n}$. Therefore

$$\begin{aligned} \mathcal{N} |n\rangle &= n |n\rangle \\ a |0\rangle &= 0 \\ a |n\rangle &= \sqrt{n} |n-1\rangle \\ a^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle \end{aligned} \quad [I-26]$$

which leads to the powerful **state vector generating rule** -- viz.

$$|n\rangle = \frac{a^\dagger^n}{\sqrt{n!}} |0\rangle \quad [I-27]$$

There is another interest connect between the two alternative treatments of a harmonic oscillator: we may use Equations [I-26] and [I-27] to obtain the coordinate representatives of the harmonic oscillator states. Using Equation [I-15] we see that

$$\begin{aligned} \langle q|a |0\rangle &= \sqrt{\frac{m}{2\hbar}} \langle q| [q + i p / m] |0\rangle \\ &= \sqrt{\frac{m}{2\hbar}} \left(q + \frac{\hbar}{m} \frac{d}{dq} \right) \langle q|0\rangle = 0 \end{aligned} \quad [I-28]$$

Therefore $\langle q|0\rangle = c_0 \exp -\frac{m}{2\hbar} q^2$ [I-29]

and with the equivalence

$$a^\dagger = \sqrt{\frac{m}{2\hbar}} \left(q - \frac{\hbar}{m} \frac{d}{dq} \right) \quad [I-30]$$

Equation [I-27] yields

$$\langle q|n\rangle = \frac{1}{\sqrt{n!}} \left(\sqrt{\frac{m}{2\hbar}} \right)^n \left(q - \frac{\hbar}{m} \frac{d}{dq} \right)^n \langle q|0\rangle \quad [I-31]$$

which is the generator of the eigenfunction displayed in Equation [I-10a].

The connection between bosons and harmonic oscillators:

There are two distinct interpretations of the energy formula $\mathcal{E}_n = \hbar \left(n + \frac{1}{2} \right)$:

- a. The formula describes the energy eigenvalue which corresponds to a given eigenstate of a particular harmonic oscillator.
- b. The formula describes the total energy of a system of n identical noninteracting quanta (particles), each of which is in the same dynamic state. The energy of the particle state is \hbar .

Again we turn to Dirac⁴ who rigorously articulates the equivalence of these two view points. To quote his conclusion ".....**This means that the dynamic system consisting of an assembly of similar bosons is equivalent to the dynamic system consisting of a set of oscillators - the two systems are just the same system looked at from two different points of view. There is one oscillator associated with each independent boson state. We have here one of the most fundamental results of quantum mechanics, which enables a unification of the wave and corpuscular theories of light to be effected.....Thus a set of harmonic oscillators is equivalent to an assembly of bosons in stationary states with no interactions between**

⁴ In Sections 60 and 61 of P. A. M. Dirac's *The Principles of Quantum Mechanics* (Revised fourth edition), Oxford University Press (1967).

them. If an oscillator of the set is in its n'th quantum state, there are n' bosons in the associated boson state.