5) Now we turn to <u>Topic II</u> on p. QF1 -- i.e. quantization of A_μ. We do this by analogy with the well-known QM of the simple harmonic oscillator (SHO). The exercise provides a natural context for the "photon" concept. The reason for invoking the SHO is that the "normal modes" of the EM radiation field can be thought of -- by means of Fourier's Theorem -- as a continuous distribution of elementary oscillators.

Single-mode, standing-wave realization of the EM field. [Davydov, ¶ 80].

Define terms...

(1) $\mathbb{k}$ = wave vector , $k = |\mathbb{k}|$ = wave number $\left\{ \begin{array}{l} \text{wavelength} : \lambda = 2\pi/k, \\ \measuredangle\text{lar freq.} : \omega = kc. \end{array} \right.$ (15a)

(2) $\hat{\epsilon}$ = unit polarization vector $\left\{ \begin{array}{l} \hat{\epsilon} = \text{unit vector in direction of } \mathbb{E}_r. \ \underline{\text{NOTE}}: \text{there} \\ \text{are } \underline{\text{two}} \text{ indep}^{\underline{t}} \text{ polarizations for each transverse wave.} \end{array} \right.$ (15b)

(3) Drop subscript "r" for the radiation fields. All fields calculated henceforth are exclusively free radiation fields (no sources present, etc.)*

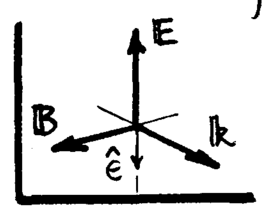
To begin, consider vector potential for a <u>standing</u> EM wave at wave vector $\mathbb{k}$ and polarization $\hat{\epsilon}$ (a single mode); it is...

$$\rightarrow \mathbb{A} = \hat{\epsilon}\,\zeta \cos(\mathbb{k}\cdot\mathbb{r}), \text{ obeying} : (\nabla^2 + k^2)\,\mathbb{A} = 0, \text{ standing wave eqtn.} \quad (16)$$

The amplitude ζ of $\mathbb{A}$, which is arbitrary in time, turns out to be the generalized "position" coordinate for this elementary EM field oscillator.

For a free radiation field, we can choose $\phi = 0$ & $\nabla\cdot\mathbb{A} = 0$ (Coulomb gauge). Then the fields accompanying $\mathbb{A}$ of Eq. (16) are:

$$\left.\begin{array}{l} \text{electric field} : \mathbb{E} = -\frac{1}{c}\,\partial\mathbb{A}/\partial t = -\hat{\epsilon}\,(\dot{\zeta}/c)\cos(\mathbb{k}\cdot\mathbb{r}); \\ \text{magnetic field} : \mathbb{B} = \nabla\times\mathbb{A} = -(\mathbb{k}\times\hat{\epsilon})\,\zeta\sin(\mathbb{k}\cdot\mathbb{r}). \end{array}\right\} \quad (17)$$



We have a <u>transverse</u> EM wave, since $\mathbb{E}\cdot\mathbb{B} = 0$, and both fields are $\perp \mathbb{k}$. The directions $\mathbb{k}$, $\mathbb{E}$ & $\mathbb{B}$ are mutually $\perp$.

The energy density of the standing wave in Eq. (17) is, locally...

$$\rightarrow U = \frac{1}{8\pi}(\mathbb{E}^2 + \mathbb{B}^2) = \frac{1}{8\pi}\left[(\dot{\zeta}/c)^2\cos^2(\mathbb{k}\cdot\mathbb{r}) + k^2\zeta^2\sin^2(\mathbb{k}\cdot\mathbb{r})\right]. \quad (18)$$

Over a macroscopic volume V (linear dimension $\gg \lambda = \frac{2\pi}{k}$), total field energy is:

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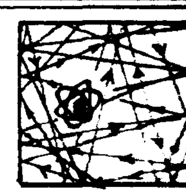
* By this time, we are thinking of the problem as that of an atom enclosed in a box with perfectly reflecting walls. Photons (radiation) in the box bounce around randomly (& freely), "bathing" the atom in $\mathbb{A}_{rad}$, etc.



Analogy: radn field energy ↔ SHO. How SHO's work.

$$\mathcal{E} = \int_V U\, d^3x \to \underset{\text{avg. value in V}}{\bar{U}}V = \frac{V}{8\pi}\Big[(\dot{\zeta}/c)^2 \underbrace{\langle\cos^2(\mathbf{k}\cdot\mathbf{r})\rangle}_{1/2,\text{ over many }\lambda's} + k^2\zeta^2 \underbrace{\langle\sin^2(\mathbf{k}\cdot\mathbf{r})\rangle}_{1/2,\text{ over many }\lambda's}\Big]$$

i.e. $$\underline{\underline{\bar{\mathcal{E}} = \frac{1}{2}\left[(V/8\pi c^2)\dot{\zeta}^2 + (Vk^2/8\pi)\zeta^2\right]}}$$ average field energy in "large" box of volume V. (19)

This expression is the direct analogue of the total energy of a SHO, as

... for SHO of mass m, natural frequency ω, and generalized position q ...

$$\underline{\underline{\mathcal{E}_{SHO} = \frac{1}{2}\left[m\dot{q}^2 + m\omega^2 q^2\right]}}.$$ (here q = coordinate, not a charge.) (20)

Evidently the two expressions are identical, if we define:

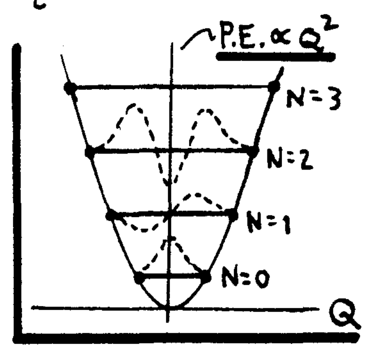
$$\boxed{\omega = kc,\ m = V/8\pi c^2,\ q = \zeta \Rightarrow \bar{\mathcal{E}} = \mathcal{E}_{SHO}}.$$ (21)

We shall take this analogy seriously, because the structure of a quantized field theory must deal with the SHO decomposition of those fields, and thus must incorporate SHO quantization to some degree. Eqs. (19)-(21) are a beginning.

ASIDE Recollections on how QM SHO's work. [Ref. Sakurai, Sec. 2.3].

1. Let Q = generalized position of the SHO motion, and $P = m\dot{Q}$ = canonical momentum.

→ Quantize SHO by imposing $[Q,P] = i\hbar$ on $H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 Q^2$. (22)



Get eigenfcns $|N\rangle$. In Q-space, these are Hermite polynomials of degree $N = 0, 1, 2, 3 \ldots$

Get eigenenergies: $\underline{\underline{E_N = \langle N|H|N\rangle = (N+\frac{1}{2})\hbar\omega}}$. (23)

NOTE: for $N=0$, get "zero-point energy": $\underline{E_0 = \frac{1}{2}\hbar\omega}$. This energy is really present, and is necessary for compatibility w/ Uncertainty Principle.

2. In the SHO state $|N\rangle$, we can say the energy is: $\underline{E_N = E_0 + \text{energy of } N \text{ quanta}}$, w/ each quantum carrying a discrete energy $\hbar\omega$. These quanta will later be

Details of SHO operation. Notion of photons.

identified with **photons**, so the SHO state $|N\rangle$ signifies there are N photons present, each with energy $\hbar\omega$. It is fair to mention photons here, because-- by Einstein's work on the photoelectric effect (ca. 1905)-- the photon had already been identified as a working quantum, carrying energy $\hbar\omega$. NOTE: even when no photons are present (i.e. $N=0$ and "vacuum state" $|0\rangle$), the mode ω still has the "zero-point" energy $E_0 = \frac{1}{2}\hbar\omega$, like half a photon there, for free. These energies are called the "zero-point oscillations" of the field, and cannot be thrown out w/o violating the Uncertainty Principle. This zero-point behavior causes Big Trouble... e.g. the overall vacuum $|0\rangle$ has ∞ energy.★

3. Some SHO matrix elements will be useful to us. They are...

$$\langle N_1|Q|N_2\rangle = \begin{cases} (\hbar/2m\omega)^{1/2}\sqrt{N}, & \text{for } N_2=N \;\&\; N_1=N-1; \\ (\hbar/2m\omega)^{1/2}\sqrt{N+1}, & \text{for } N_2=N \;\&\; N_1=N+1. \end{cases} \left(\begin{matrix}\text{and zero,}\\ \text{otherwise}\end{matrix}\right). \quad (24)$$

For matrix elements of P, use: $\dot{Q} = \frac{i}{\hbar}[H,Q] \Rightarrow P = (im/\hbar)(HQ-QH)$. So...

$$\rightarrow \langle N_1|P|N_2\rangle = \frac{im}{\hbar}\left(\langle N_1|HQ|N_2\rangle - \langle N_1|QH|N_2\rangle\right)$$

$$= im\omega(N_1-N_2)\langle N_1|Q|N_2\rangle \leftarrow \text{now use Eq. (24)}$$

$$\langle N_1|P|N_2\rangle = \begin{cases} -i(m\hbar\omega/2)^{1/2}\sqrt{N}, & \text{for } N_2=N \;\&\; N_1=N-1; \\ +i(m\hbar\omega/2)^{1/2}\sqrt{N+1}, & \text{for } N_2=N \;\&\; N_1=N+1. \end{cases} \left(\begin{matrix}\text{and zero,}\\ \text{otherwise}\end{matrix}\right). \quad (25)$$

END of ASIDE

★ E.g. the average energy of an assembly of QM SHO's at frequency ω, in thermal equilibrium at temperature T is (w/ k = Boltzmann cnst & $E_N = (N+\frac{1}{2})\hbar\omega$):

$$\bar{E}(\omega) = \left(\sum_{N=0}^{\infty} E_N e^{-E_N/kT}\right) \Big/ \left(\sum_{N=0}^{\infty} e^{-E_N/kT}\right) = \underbrace{\hbar\omega/(e^{\hbar\omega/kT}-1)}_{\text{Planck distribution}} + \underbrace{\tfrac{1}{2}\hbar\omega}_{\text{zero-point energy}}$$

The total field energy: $\int_{\omega=0}^{\omega=\infty} \bar{E}(\omega) \times \left[\begin{matrix}\#\text{modes}\\ \text{at } \omega\end{matrix}\right] \times d\omega$, then picks up a contribution from the zero-point energies which goes as $\int_0^\infty \omega^3 d\omega \to \infty$. Called an "ultraviolet catastrophe".

Field quantization via SHO. Annihilation & creation operators a & $a^\dagger$.

3) Now, to quantize the EM field in the mode ($\mathbb{k}$; $\hat{\epsilon}$), we just take over the SHO quantization verbatim. That is, where ζ is the amplitude of the field vector potential [i.e. $\mathbb{A} = \hat{\epsilon}\,\zeta \cos(\mathbb{k}\cdot\mathbb{r})$ of Eq. (16)], we define -- as in Eq. (21):

$$\left[\begin{array}{l} \zeta = q \text{, generalized position; } p = m\dot{q} = (V/8\pi c^2)\dot{\zeta} \text{, canonical mom}^{\underline{m}}; \\ kc = \omega \text{, natural frequency; } V/8\pi c^2 = m \text{, field "mass" (sic).} \end{array}\right\} \quad (26)$$

Then, imposing: $[q, p] = i\hbar$, quantizes the field energy $\bar{\mathcal{E}}$ in Eq. (19), and we get:

$$\underline{\text{field SHO}}\begin{cases} \text{eigenstates } |N\rangle \leftarrow \text{a state (at freq. } \omega\text{) with } N \text{ photons present;} \\ \text{eigenenergies : } \mathcal{E}_N = (N+\tfrac{1}{2})\hbar\omega \leftarrow \text{energy of } N \text{ photons + zero-pt.} \end{cases} \quad (27)$$

It's that simple. The field can now supply or absorb photons via $N \to N \mp 1$.

The idea of emission & absorption of photons by the field via a change $N \to N \mp 1$ in the photon occupation number now finds a beautifully clear representation in the "ladder operators" a & $a^\dagger$ of the SHO. We define:

$$\boxed{\begin{array}{l} a = (Vk/16\pi\hbar c)^{1/2}\zeta + i(4\pi c/V\hbar k)^{1/2} p \\ a^\dagger = (\quad \text{"} \quad)^{1/2}\zeta - i(\quad \text{"} \quad)^{1/2} p \end{array}} \begin{array}{l} \leftarrow \text{step-down (annihilation) operator;} \\ \leftarrow \text{step-up (creation) operator.} \end{array} \quad (28)$$

The SHO quantization condition: $[q, p] = i\hbar$, is now replaced by: $\underline{[a, a^\dagger] = 1}$ (Sakurai, Eqs. (2.3.2) & (2.3.3), etc). Only nonvanishing matrix elements are...

$$\left\|\begin{array}{ll} \langle N-1|a|N\rangle = \sqrt{N}, \text{ i.e. } \underline{\underline{a|N\rangle = \sqrt{N}\,|N-1\rangle}} & \text{a steps-down by one quantum, field loses one photon;} \\ \langle N+1|a^\dagger|N\rangle = \sqrt{N+1}, \text{ i.e. } \underline{\underline{a^\dagger|N\rangle = \sqrt{N+1}\,|N+1\rangle}} & a^\dagger \text{ steps-up by one quantum, field gains one photon.} \end{array}\right. \quad (29)$$

Here the notion of the field emitting (i.e. supplying) or absorbing photons is born... these are just processes where a or $a^\dagger$ operate on the field SHO states $|N\rangle$ of Eq. (27), supplying or absorbing a quantum of energy $\hbar\omega$.

Quantized radiation field as an operator. Matrix elements of $\mathcal{H}_{int}$.

With this quantization scheme, we can now say the radiation field is quantized in the mode $(\mathbf{k};\hat{\epsilon})$ because all its transactions with other (quantum) systems will occur in terms of discrete quanta (photons) of energy $\hbar\omega$. The field quantities themselves become operators, as follows. The inverse of Eqs. (28) give the "position" ζ and "momentum" $p = m\dot{\zeta}$ of $\mathbb{A}$ as...

$$\zeta = (4\pi\hbar c/Vk)^{1/2}(a^\dagger + a), \quad p = i(V\hbar k/16\pi c)^{1/2}(a^\dagger - a);$$

So//

$$\mathbb{A} = \hat{\epsilon}\,\zeta\cos(\mathbf{k}\cdot\mathbf{r}) = \left(\frac{4\pi\hbar c}{Vk}\right)^{\frac{1}{2}}\hat{\epsilon}\,(a^\dagger + a)\cos(\mathbf{k}\cdot\mathbf{r}). \tag{30}$$

The $a^\dagger$ & a do not operate on the (atom's) space coordinate $\mathbf{r}$; they just operate on the photon states $|N\rangle$ in the field. Then it is clear that $\mathbb{A}$ is an operator, in that $\mathbb{A}|N\rangle$ will generate states $|N\pm 1\rangle$ in the field.

Now, when matrix elements of $\mathcal{H}_{int} \sim \mathbb{A}\binom{\text{radn}}{\text{fld}} \cdot \mathbb{p}\binom{\text{charge}}{\text{motion}}$ [see Eq. (11b)] are taken w.r.t. direct product states $|n(\text{atom})(N(\text{photons}))\rangle$ [see Eq. (12)], as indicated in the theory sketch in Eq. (14), we have a mechanism for ensuring that $\langle m(M)|\mathcal{H}_{int}|n(N)\rangle \sim \langle(M)|\mathbb{A}|(N)\rangle\cdot\langle m|\mathbb{p}|n\rangle$ will properly describe $n\rightarrow m$ for the atom, with $N\rightarrow M = N\pm 1$ for the field interpreted as the emission or absorption of a photon during the transition.

We have work to do to generalize these notions. At this point, we have only quantized the standing wave $(\mathbf{k};\hat{\epsilon})$ vector potential $\mathbb{A}$ of Eq. (30). We need to put in time dependence, to get traveling waves, and we should generalize to a $\mathbf{k}$-spectrum for arbitrary photon fields. This is ~ straightforward.

In passing, we note the field Hamiltonian for freq. ω can be written

$$\rightarrow \mathcal{H}_\omega = (a^\dagger a + \tfrac{1}{2})\hbar\omega\,; \quad {}^{\text{w/}}\ \underline{\underline{a^\dagger a = N}}\ (\text{w.r.t. } |N\rangle), \ \underline{\underline{\text{the number operator}}}. \tag{31}$$

This comes in handy, later, when we track the field energy.