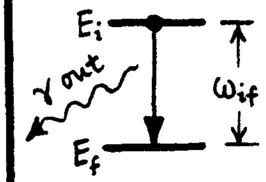
EM field as part of a quantum system.

Ref. UC notes, 1961

Interaction of a Quantum System w/ a Quantized EM Field

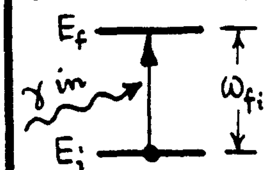
In our discussion of time-dependent perturbation theory, it was natural to speak of transitions $i \to f$ in a quantum system as being either "emission" or "absorption" processes, wherein a "photon" of energy $\simeq \hbar|\omega_{if}|$ was either given-up-to or gained-from some external field. The external field is of course Maxwell's EM field, and now we shall study why the above language is sensible.

EMISSION



photon OUT @ energy $\mathcal{E}_\gamma \simeq \hbar\omega_{if}$

ABSORPTION



photon IN @ energy $\mathcal{E}_\gamma \simeq \hbar\omega_{fi}$

Instead of separating the quantum system (say an atom) from the external field, we shall consider the whole works, atom plus field, to be our quantum system... we do this in part because we want to be able to accurately track energy transfers between atom & field. The EM field, now as part of the overall "quantum system", itself becomes quantized -- in just such a way that it can absorb the quantized energy $\hbar\omega_{if}$ when the atom emits it, or emit $\hbar\omega_{fi}$ when the atom absorbs it. These quantized energies $\hbar|\omega_{if}|$ are "photons", and the field needs some quantum structure to be able to trade its photons with the (quantized) atom.

The most interesting feature of the theory is the notion of a quantized EM field. Field quantization is achieved by viewing the field as a (continuous) assembly of SHO's (via Fourier: $\mathbf{E}(\mathbf{r},t) = \int dt \int d^3x\, \tilde{\mathbf{E}}(\mathbf{k},\omega)\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$), then quantizing each mode $(\omega,\mathbf{k})$ via the "well-known" rules for SHO quantization. We will use the annihilation (a) - creation ($a^\dagger$) operator formalism for the field SHO's [Sakurai: 2.3].

Our discussion is in 3 steps, viz.

I. Interaction of a charged particle with an EM field.

II. Quantization of the radiation field & role of "photons".

III. Calculation of transition amplitudes for the atom-field system.

Nonrelativistic (q,m) in EM potentials $(\phi, \mathbb{A})$.

1) From classical electrodynamics, the electric & magnetic fields $\mathbb{E}$ & $\mathbb{B}$ are derivable from scalar & vector potentials ϕ & $\mathbb{A}$ as [Jackson, Eq. (6.31)]★

$$\rightarrow \mathbb{E} = -\nabla\phi - \frac{1}{c}(\partial\mathbb{A}/\partial t), \quad \mathbb{B} = \nabla\times\mathbb{A}. \tag{1}$$

Also the (nonrelativistic) Hamiltonian for a particle (q,m) in $(\phi, \mathbb{A})$ is¶:

$$\rightarrow \mathcal{H}_{EM} = \frac{1}{2m}\left(\mathbb{p} - \frac{q}{c}\mathbb{A}\right)^2 + q\phi. \tag{2}$$

$\boxed{\text{REMARKS}}$ on $\mathcal{H}_{EM}$.

1. $\mathbb{p}$ is not the usual particle momentum. In fact: $\mathbb{p} = m\mathbb{v} + (q/c)\mathbb{A}$, is the sum of the usual particle mechanical momentum and a correction due to the field.
2. But $\mathbb{p}$ is the momentum which is canonical for position $\mathbb{r}$, in that Hamilton's eqtns of motion lead to the correct Lorentz force law, i.e.

$$\frac{\partial}{\partial\mathbb{r}}\mathcal{H}_{EM} = (-)\frac{d}{dt}\mathbb{p} \Rightarrow \frac{d}{dt}(m\mathbb{v}) = q\left(\mathbb{E} + \frac{\mathbb{v}}{c}\times\mathbb{B}\right). \tag{3}$$

3. It is the canonical momentum $\mathbb{p}$ (and not $m\mathbb{v}$) which will be replaced by the operator $(-)i\hbar\nabla$ when we do the QM on (q,m).

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2) We assume the EM field in $\mathcal{H}_{EM}$ can be split into two parts, which we shall discuss and treat separately. Namely...

$$\rightarrow (\phi, \mathbb{A}) = \overset{①}{(\phi, \mathbb{A})_{ext.}} + \overset{②}{(\phi, \mathbb{A})_{rad}}. \tag{4}$$

① ⇒ external static fields (to be treated classically), e.g. ϕ_{ext} = Coulomb potential, $\mathbb{A}_{ext} \doteq \frac{1}{2}\mathbb{B}_{ext}\times\mathbb{r}$ (Zeeman field). We choose $\mathbb{A}_{ext}=0$, and set $q\phi_{ext} = V$.

② ⇒ radiation fields (to be quantized). These obey the free-field wave eqtn, viz: $\left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\mathbb{A}_{rad} = 0$, $\phi_{rad} = 0$. We choose the Coulomb gauge: $\nabla\cdot\mathbb{A}_{rad} = 0$, which describes the propagation of transverse EM waves [Jackson, Sec. 6.5].

¶ Jackson Eq. (12.14). $\mathcal{H}_{EM}$ of Eq. (2) is correct through terms of $O(1/c^2)$.

★ References are to J.D. Jackson "Classical Electrodynamics" (Wiley, 2nd ed., 1975).

Reduction of $\mathcal{H}_{EM}$ to binding + coupling terms.

With these choices, $\mathcal{H}_{EM}$ of Eq. (2) becomes...

$$\rightarrow \mathcal{H}_{EM} = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbb{A}_r\right)^2 + V \quad \leftarrow \mathbb{A}_r \text{ is } \mathbb{A}_{rad} \text{ for the radiation field}$$

$$= \underbrace{\left(\frac{1}{2m}\mathbf{p}^2 + V\right)}_{①} - \underbrace{\frac{q}{2mc}\left(\mathbf{p}\cdot\mathbb{A}_r + \mathbb{A}_r\cdot\mathbf{p}\right)}_{②} + \underbrace{\frac{q^2}{2mc^2}\mathbb{A}_r^2}_{③}. \tag{5}$$

①: With $\mathbf{p} \rightarrow (-)i\hbar\nabla$, this is the usual Schrödinger Hamiltonian; denote it by:

$$\underline{\underline{\mathcal{H}_S = \frac{1}{2m}\mathbf{p}^2 + V}}. \tag{6}$$

$\mathcal{H}_S$ generates a bound quantum system for (q, m). Assume solutions: $\mathcal{H}_S\,\phi_n(\mathbf{r}) = E_n\,\phi_n(\mathbf{r})$, known.

②: This is the coupling between the bound particle (q,m) and the radiation field. Ultimately $\mathbb{A}_r$ will be quantized. For now, note that with $\mathbf{p} \rightarrow (-)i\hbar\nabla$...

$$(\mathbf{p}\cdot\mathbb{A}_r + \mathbb{A}_r\cdot\mathbf{p})\psi = -i\hbar\left[\nabla\cdot(\mathbb{A}_r\psi) + \mathbb{A}_r\cdot(\nabla\psi)\right]$$

$$= -i\hbar\underbrace{(\nabla\cdot\mathbb{A}_r)}_{0,\text{ by choice of Coulomb gauge}}\psi + 2\,\mathbb{A}_r\cdot\mathbf{p}\,\psi$$

So

$$\underline{\underline{\mathbf{p}\cdot\mathbb{A}_r + \mathbb{A}_r\cdot\mathbf{p} = 2\,\mathbb{A}_r\cdot\mathbf{p}}}, \quad \text{w.r.t. wavefcns } \psi. \tag{7}$$

③: We shall ignore this term as "small". We note: term③/term② $\sim qA_r/cp$. If A_r is generated by motion of q in an atom of size a_0, then $A_r \sim qv/ca_0$, and the ratio: ③/② $\sim (q^2/a_0)/mc^2 \sim$ (atom binding energy)/(rest energy) $\ll 1$. Term ③ is important only when (q,m) is subjected to intense external (laser) fields.

At this point, we have reduced $\mathcal{H}_{EM}$ to just two terms, viz

$$\boxed{\mathcal{H}_{EM} = \mathcal{H}_S - (q/mc)\,\mathbb{A}_r\cdot\mathbf{p}}. \tag{8}$$

This is not the entire Hamiltonian for the system: atom + field, but it does represent the particle binding, through $\mathcal{H}_S$, and the coupling of the (spinless) particle's motion to the radiation field, through $\mathbb{A}_r\cdot\mathbf{p}$.

Total System Hamiltonian: atom + field. Anticipation of the theory.

3) Two add-ons to the total system (atom + field) Hamiltonian...

A. Suppose q has spin $\frac{1}{2}$, and thus a magnetic moment $\boldsymbol{\mu} = \underbrace{\left(\frac{q\hbar}{2mc}\right)}_{\text{Bohr magneton}} \boldsymbol{\sigma} = \left(\frac{q}{mc}\right)\mathbf{S}$.
$\boldsymbol{\mu}$ couples to the radiation magnetic field $\mathbf{B}_r$ as...

$$\rightarrow \mathcal{H}_{mag} = -\boldsymbol{\mu}\cdot\mathbf{B}_r = -(q/mc)\,\mathbf{S}\cdot\mathbf{B}_r. \tag{9}$$

B. The energy in the radiation field itself should be included. It is...

$$\rightarrow \mathcal{H}_r = \int d^3x\, \frac{1}{8\pi}\left(\mathbf{E}_r^2 + \mathbf{B}_r^2\right), \text{ classically [Jackson, Eq. (6.112)]}. \tag{10}$$

Later, QMly, this will be a sum $\sum_\omega (N_\omega + \frac{1}{2})\hbar\omega$ over photon energies $\hbar\omega$.

With these add-ons, we take as the total system (atom + field) Hamiltonian...

$$\rightarrow \underline{\mathcal{H} = \mathcal{H}_{EM} + \mathcal{H}_{mag} + \mathcal{H}_r = \mathcal{H}_0 + \mathcal{H}_{int}}; \tag{11a}$$

$$\left[\begin{array}{ll} \text{w/} \; \mathcal{H}_0 = \mathcal{H}_s + \mathcal{H}_r & \int \begin{array}{l}\mathcal{H}_s \Rightarrow \text{unperturbed bound system (atom) [Eq. (6)]},\\ \mathcal{H}_r \Rightarrow \text{free radiation field (photons) [Eq. (10)]}\end{array} \\ \text{and/} \; \mathcal{H}_{int} = -(q/mc)\left[\mathbf{A}_r\cdot\mathbf{p} + \mathbf{S}\cdot\mathbf{B}_r\right] & \int \text{coupling between atom and field. [Eqs. (8) \& (9)]} \end{array}\right] \tag{11b}$$

This formulation completes Topic I as listed on p. QF 1 above.

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4) Before treating Topic II, we anticipate how the QM treatment of the overall system (atom + field) in Eqs. (11) can be developed. Quantization of the atom is "obvious"; we take it on faith that the field will be quantized in terms of SHO's at frequencies ω... where the energy in mode ω is $(N_\omega + \frac{1}{2})\hbar\omega$, and $N_\omega = 0, 1, 2, \ldots$ can be interpreted as the # "photons" in that mode. Then...

1. Let $\{\phi_n(\mathbf{r})\}$ be the eigenfcns of $\mathcal{H}_s$, i.e.: $\mathcal{H}_s\phi_n(\mathbf{r}) = E_n\phi_n(\mathbf{r})$. ← ATOM.
Let $|(N_\omega)\rangle = |\ldots N_\omega \ldots\rangle$ " " $\mathcal{H}_r$, i.e.: $\mathcal{H}_r|(N_\omega)\rangle = \mathcal{E}_{(N)}|(N_\omega)\rangle$. ← FIELD.

Then eigenfcns of $\mathcal{H}_0 = \mathcal{H}_s + \mathcal{H}_r$ are the direct product states:

$$\rightarrow |n(N_\omega)\rangle = \phi_n(\mathbf{r})\,|\ldots N_\omega \ldots\rangle \longleftrightarrow \text{eigenvalues } (E_n + \mathcal{E}_{(N)}) \text{ of } \mathcal{H}_0 \tag{12}$$

Interaction representation for atom + field system.

Here: $\mathcal{E}_{(N)} = \sum_{\omega} (N_\omega + \frac{1}{2})\hbar\omega$, is the total energy (by photon counting) in the radⁿ fld.

2. Use the direct product states of Eq. (12) as a basis when the coupling $\mathcal{H}_{int}$ is turned on. The most general state of (atom + field) is the superposition:

$$\rightarrow \psi(t) = \sum_{n(N)} C_{n(N)}(t)\,|n(N)\rangle\, e^{-(i/\hbar)E_{n(N)}t}, \quad \underline{N = \#\text{ photons at freq. } \omega}. \tag{13}$$

(we've dropped the subscript "ω" on N). With this ψ, the Schrödinger wave eqtn: $i\hbar\,\partial\psi/\partial t = (\mathcal{H}_0 + \mathcal{H}_{int})\psi$, then gives -- exactly

$$\boxed{i\hbar\,\dot{C}_{m(M)}(t) = \sum_{n(N)} C_{n(N)}(t)\,\langle m(M)|\,\mathcal{H}_{int}\,|n(N)\rangle\, e^{\frac{i}{\hbar}(E_{m(M)} - E_{n(N)})t}}, \tag{14}$$

w/ $E_{n(N)} = E_n + \mathcal{E}_{(N)}$ is total system energy, with atom at energy E_n, and radiation field with a distribution of (N) photons present [i.e. N_1 photons at ω_1, N_2 photons at ω_2, etc.]. An eqtn of the <u>form</u> of (14) was the starting point for our treatment of time-dependent perturbation theory (see class notes, p. tD3); there, as here, it was <u>exact</u>. The coefficients $|C_{n(N)}|^2$ are interpreted as the probabilities of actually finding the state $|n(N)\rangle$ at energy $E_{n(N)}$.

3. A perturbation theory on Eq. (14) will yield "transition amplitudes", for changes in the overall system, when $i(I) \rightarrow f(F)$, with the atom making a transition from an initial state i to a final state f, while the state of the radiation field changes $(I) \rightarrow (F)$. Overall, system energy must be conserved: if $i \rightarrow f$ gains (loses) energy, then $(I) \rightarrow (F)$ must lose (gain) energy.