The QED Hamiltonian

- rigorous derivation from first principles
  Ref. API, Appendix
- $\simeq$ 100 equations ∇
  BUT: result is simple and intuitive
  (e.g. $\vec{E}\cdot\vec{d}$ electric dipole interaction)

To learn from this treatment

CLASSICAL
- How to rigorously separate "local" Coulomb fields from radiation field
- To identify the truly independent degrees of freedom
- After deriving the appropriate classical description, quantization is straightforward
- Rigorous derivation of electric dipole Hamiltonian INCLUDING the A^2 term

QED

- Maxwell eq.

$$\nabla \cdot \mathbf{E}(\mathbf{r}, t) = \frac{1}{\varepsilon_0} \rho(\mathbf{r}, t) \tag{1.a}$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0 \tag{1.b}$$

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{r}, t) \tag{1.c}$$

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \frac{1}{c^2} \frac{\partial}{\partial t} \mathbf{E}(\mathbf{r}, t) + \frac{1}{\varepsilon_0 c^2} \mathbf{j}(\mathbf{r}, t) \tag{1.d}$$

Six Field Components

- Spatial Fourier transform

$$i\mathbf{k} \cdot \mathscr{E}(\mathbf{k}, t) = \frac{1}{\varepsilon_0} \rho(\mathbf{k}, t) \tag{2.a}$$

$$i\mathbf{k} \cdot \mathscr{B}(\mathbf{k}, t) = 0 \tag{2.b}$$

Longitudinal

$$i\mathbf{k} \times \mathscr{E}(\mathbf{k}, t) = -\frac{\partial}{\partial t} \mathscr{B}(\mathbf{k}, t) \tag{2.c}$$

$$i\mathbf{k} \times \mathscr{B}(\mathbf{k}, t) = \frac{1}{c^2} \frac{\partial \mathscr{E}(\mathbf{k}, t)}{\partial t} + \frac{1}{\varepsilon_0 c^2} \mathscr{j}(\mathbf{k}, t) \tag{2.d}$$

transverse

Fourier transform allows us to rigorously separate $E_\parallel, B_\parallel$ from $E_\perp, B_\perp$

- transverse and Long. field decouple

$$\mathbf{E}_\parallel(\mathbf{r}, t) = \frac{-1}{4\pi\varepsilon_0} \int d^3r' \, \rho(\mathbf{r}', t) \nabla_{\mathbf{r}} \frac{1}{|\mathbf{r} - \mathbf{r}'|} \tag{5.a}$$

$$\mathbf{B}_\parallel(\mathbf{r}, t) = 0. \tag{5.b}$$

expressed by momentary position of charges

$E_\parallel$ is not independent variable

$$\frac{\partial}{\partial t} \mathscr{B}(\mathbf{k}, t) = -i\mathbf{k} \times \mathscr{E}_\perp(\mathbf{k}, t) \tag{6.a}$$

$$\frac{\partial}{\partial t} \mathscr{E}_\perp(\mathbf{k}, t) = c^2 i\mathbf{k} \times \mathscr{B}(\mathbf{k}, t) - \frac{1}{\varepsilon_0} \mathscr{j}_\perp(\mathbf{k}, t). \tag{6.b}$$

Vector Potential

$$\mathbf{E}(\mathbf{r},t) = -\nabla U(\mathbf{r},t) - \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t} \tag{7.a}$$

$$\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t) \tag{7.b}$$

$$\mathscr{E}(\mathbf{k},t) = -i\mathbf{k}\mathscr{U}(\mathbf{k},t) - \frac{\partial \mathscr{A}(\mathbf{k},t)}{\partial t} \tag{8.a}$$

$$\mathscr{B}(\mathbf{k},t) = i\mathbf{k} \times \mathscr{A}(\mathbf{k},t). \tag{8.b}$$

Note: transverse Fields depend only on $A_\perp$

- Coulomb Gauge $\nabla \cdot A = 0$

$$A_{\parallel}(r,t) = 0$$

$$U(\mathbf{r},t) = \frac{1}{4\pi\varepsilon_0}\int \mathrm{d}^3r' \, \frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}. \tag{15}$$

$\Rightarrow$ The two components of the transverse vector potential are the independent variables of the radiation field

- Normal modes

$$\begin{aligned}\boldsymbol{\alpha}(\mathbf{k},t) &= \lambda(k)\left[\mathscr{E}_\perp(\mathbf{k},t) - c\frac{\mathbf{k}}{k}\times\mathscr{B}(\mathbf{k},t)\right] \\ &= \lambda(k)\left[-\dot{\mathscr{A}}_\perp(\mathbf{k},t) + i\omega\mathscr{A}_\perp(\mathbf{k},t)\right]\end{aligned} \tag{16}$$

$$\dot{\boldsymbol{\alpha}}(\mathbf{k},t) + i\omega\boldsymbol{\alpha}(\mathbf{k},t) = \frac{i}{\sqrt{2\varepsilon_0\hbar\omega}}\,\mathscr{j}_\perp(\mathbf{k},t). \tag{17}$$

$$\vec{A}_\perp(r) = \int d^3k \sum_{\varepsilon} A_w \left[\vec{\varepsilon}\,\alpha_\varepsilon(k)\, e^{ikr} + \vec{\varepsilon}\,\alpha_\varepsilon^*(k)\, e^{-ikr}\right]$$

Note: Field is determined by $A_\perp$ and $\dot{A}_\perp$ at $t=0$

Equation of motion couples the two components of $A_\perp$

$\Rightarrow$ Introduce decoupled normal modes

Each normal mode acts as an independent harmonic oscillator.

Let's repeat some of this derivation with a focus on energy

$$H = \sum \frac{1}{2} m_\alpha v_\alpha^2 + \underbrace{\frac{\varepsilon_0}{2}\int d^3r \left(E^2(r,t) + c^2 B^2(r,t)\right)}$$

$$\rightarrow \underbrace{\frac{\varepsilon_0}{2}\int d^3r\, E_\parallel^2}_{\text{given by Coulomb integral}} + \underbrace{\frac{\varepsilon_0}{2}\int d^3r \left(E_\perp^2 + c^2 B^2\right)}_{\text{energy of the radiation field } H_{trans}}$$

given by Coulomb integral

$$\frac{1}{8\pi\varepsilon_0}\iint d^3r\, d^3r'\, \frac{\rho(r)\rho(r')}{|r-r'|}$$

will be split into self-energy and interaction energy

energy of the radiation field H_{trans}

$$H_{trans} = \varepsilon_0 \sum_{\varepsilon} \int d^3k \left[\frac{\pi_\varepsilon^* \pi}{\varepsilon_0^2} + c^2 k^2 A_\varepsilon^* A_\varepsilon\right] \quad *$$

$\uparrow$ Polarization

Where $\pi_\varepsilon(\mathfrak{r}) = \varepsilon_0 \dot{A}_\varepsilon(\mathfrak{r})$ conjugate momentum

normal modes

$$\alpha = (\ ) \left[-\dot{A}_\perp + i\omega A_\perp \right]$$

$$\Rightarrow H_{trans} = \int d^3k \sum_\varepsilon \frac{\hbar\omega}{2} \left[\alpha^*_\varepsilon \alpha_\varepsilon + \alpha_\varepsilon \alpha^*_\varepsilon \right] \ *$$

Both eq. * look like an HO

So far: purely classical !

Note: $\hbar$ enters only through the constant in the definition of the normal mode parameter α

See also Photons & Atoms, p. 27

Field Quantization

$$\pi_\varepsilon(k) = \varepsilon_0 \dot{A}_\varepsilon(k)$$ conjugate moment

$$[\mathscr{A}_\varepsilon(\mathbf{k}), \pi^+_{\varepsilon'}(\mathbf{k}')] = i\hbar\delta_{\varepsilon\varepsilon'}\delta(\mathbf{k}-\mathbf{k}'). \tag{20.a}$$

postulate either commutator For A and π, or For a, a^+

$$[a_\varepsilon(\mathbf{k}), a^+_{\varepsilon'}(\mathbf{k}')] = \delta_{\varepsilon\varepsilon'}\delta(\mathbf{k}-\mathbf{k}') \tag{20.b}$$

Crucial: Elimination of redundant variables is crucial BEFORE quantization: $[A_i(r), \pi_j(r')] \neq i\hbar\,\delta(r-r')$ For $i = x, y, z$

- Quantum fields

$$\mathbf{A}_\perp(\mathbf{r}) = \int \mathrm{d}^3k \sum_\varepsilon \mathscr{A}_\omega\left[\boldsymbol{\varepsilon} a_\varepsilon(\mathbf{k})\,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} + \boldsymbol{\varepsilon} a^+_\varepsilon(\mathbf{k})\,\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{21}$$

$$\mathbf{E}_\perp(\mathbf{r}) = \int \mathrm{d}^3k \sum_\varepsilon i\mathscr{E}_\omega\left[\boldsymbol{\varepsilon} a_\varepsilon(\mathbf{k})\,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} - \boldsymbol{\varepsilon} a^+_\varepsilon(\mathbf{k})\,\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{22}$$

$$\mathbf{B}(\mathbf{r}) = \int \mathrm{d}^3k \sum_\varepsilon i\mathscr{B}_\omega\left[(\boldsymbol{\kappa}\times\boldsymbol{\varepsilon}) a_\varepsilon(\mathbf{k})\,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} - (\boldsymbol{\kappa}\times\boldsymbol{\varepsilon}) a^+_\varepsilon(\mathbf{k})\,\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\right] \tag{23}$$

- Particle Operators

$$[r_i, p_j] = i\hbar\,\delta_{ij}$$

$$m_\alpha \mathbf{v}_\alpha = \mathbf{p}_\alpha - q_\alpha \mathbf{A}_\perp(\mathbf{r}_\alpha) \tag{37}$$

$$\rho(\mathbf{r}) = \sum_\alpha q_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha) \tag{38.a}$$

$$\mathbf{j}(\mathbf{r}) = \sum_\alpha q_\alpha \mathbf{v}_\alpha \delta(\mathbf{r}-\mathbf{r}_\alpha). \tag{38.b}$$

• Hamiltonian

$$H = \sum_\alpha \frac{1}{2m_\alpha}\left[\mathbf{p}_\alpha - q_\alpha \mathbf{A}_\perp(\mathbf{r}_\alpha)\right]^2 + + \sum_\alpha \underbrace{\left(-g_\alpha \frac{q_\alpha}{2m_\alpha}\right)}\mathbf{S}_\alpha \cdot \mathbf{B}(\mathbf{r}_\alpha) + V_{\text{Coul}} + H_R. \tag{40}$$

heuristically added; for e^-: derived from nonrelativistic limit of Dirac eq.

$$V_{\text{Coul}} = \frac{\varepsilon_0}{2}\int \mathrm{d}^3r\, \mathbf{E}_\parallel^2(\mathbf{r}) = \frac{\varepsilon_0}{2}\int \mathrm{d}^3k\, |\mathscr{E}_\parallel(\mathbf{k})|^2 \tag{41}$$

$$V_{\text{Coul}} = \frac{1}{2\varepsilon_0}\int \mathrm{d}^3k\, \frac{\rho^*(\mathbf{k})\rho(\mathbf{k})}{k^2} = \sum_\alpha \varepsilon_{\text{Coul}}^\alpha + \frac{1}{8\pi\varepsilon_0}\sum_{\alpha\neq\beta}\frac{q_\alpha q_\beta}{|\mathbf{r}_\alpha - \mathbf{r}_\beta|}. \tag{42}$$

$$\varepsilon_{\text{Coul}}^\alpha = \frac{q_\alpha^2}{2\varepsilon_0}\int \frac{\mathrm{d}^3k}{(2\pi)^3 k^2} = \frac{q_\alpha^2}{4\varepsilon_0\pi^2}\int_0^{k_c}\mathrm{d}k = \frac{q_\alpha^2 k_c}{4\varepsilon_0\pi^2}. \tag{43}$$

Coulomb self energy

$$H_R = \frac{\varepsilon_0}{2}\int \mathrm{d}^3r\left[\mathbf{E}_\perp^2(\mathbf{r}) + c^2\mathbf{B}^2(\mathbf{r})\right] \tag{44}$$

$$H_R = \sum_i \hbar\omega_i\left(a_i^+ a_i + \tfrac{1}{2}\right). \tag{45}$$

$(N_i + \frac{1}{2})$

• Splitting the Hamiltonian

$$H = H_P + H_R + H_I \tag{49}$$

$$H_P = \sum_\alpha \frac{\mathbf{p}_\alpha^2}{2m_\alpha} + V_{\text{Coul}} \tag{50}$$

$$H_I = H_{I1} + H_{I2} + H_{I1}^S \tag{51}$$

$$H_{I1} = -\sum_\alpha \frac{q_\alpha}{m_\alpha} \mathbf{p}_\alpha \cdot \mathbf{A}_\perp(\mathbf{r}_\alpha) \tag{52}$$

$$H_{I1}^S = -\sum_\alpha g_\alpha \frac{q_\alpha}{2m_\alpha} \mathbf{S}_\alpha \cdot \mathbf{B}(\mathbf{r}_\alpha) \tag{53}$$

$$H_{I2} = \sum_\alpha \frac{q_\alpha^2}{2m_\alpha} \mathbf{A}_\perp^2(\mathbf{r}_\alpha). \tag{54}$$

2nd order in A

Electric Dipole Approx.

$r \ll \lambda$

$$H = \sum_\alpha \frac{1}{2m_\alpha}[\mathbf{p}_\alpha - q_\alpha \mathbf{A}_\perp(0)]^2 + V_{\text{Coul}} + \sum_j \hbar\omega_j\left(a_j^+ a_j + \tfrac{1}{2}\right). \quad (71)$$

$$\vec{d} = \sum_\alpha q_\alpha \vec{r}_\alpha$$

$$T = \exp\left[-\frac{i}{\hbar}\mathbf{d}\cdot\mathbf{A}_\perp(0)\right] = \exp\left\{\sum_j (\lambda_j^* a_j - \lambda_j a_j^+)\right\} \quad (72)$$

$$\begin{aligned} H' &= THT^+ \\ &= \sum_\alpha \frac{\mathbf{p}_\alpha^2}{2m_\alpha} + V_{\text{Coul}} + \varepsilon_{\text{dip}} + \sum_j \hbar\omega_j\left(a_j^+ a_j + \tfrac{1}{2}\right) - \\ &\quad - \mathbf{d}\cdot\sum_j \mathscr{E}_{\omega_j}\left[i a_j \boldsymbol{\varepsilon}_j - i a_j^+ \boldsymbol{\varepsilon}_j\right] \end{aligned} \quad (75)$$

After transformation: no A^2 term

$$\varepsilon_{\text{dip}} = \sum_j \frac{1}{2\varepsilon_0 L^3}(\boldsymbol{\varepsilon}_j \cdot \mathbf{d})^2. \quad (76)$$

$$\mathbf{v}'_\alpha = T\mathbf{v}_\alpha T^+ = \frac{\mathbf{p}_\alpha}{m_\alpha} \quad (78)$$

$$H' = THT^{+}$$

$$= \sum_{\alpha} \frac{\mathbf{p}_{\alpha}^{2}}{2m_{\alpha}} + V_{\text{Coul}} + \varepsilon_{\text{dip}} + \sum_{j} \hbar\omega_{j}\left(a_{j}^{+}a_{j} + \tfrac{1}{2}\right) -$$

$$- \mathbf{d} \cdot \sum_{j} \mathscr{E}_{\omega_{j}}\left[ia_{j}\boldsymbol{\varepsilon}_{j} - ia_{j}^{+}\boldsymbol{\varepsilon}_{j}\right] \tag{75}$$

$$\varepsilon_{\text{dip}} = \sum_{j} \frac{1}{2\varepsilon_{0}L^{3}}\left(\boldsymbol{\varepsilon}_{j} \cdot \mathbf{d}\right)^{2}. \tag{76}$$

$$\mathbf{v}_{\alpha}' = T\mathbf{v}_{\alpha}T^{+} = \frac{\mathbf{p}_{\alpha}}{m_{\alpha}} \tag{78}$$

$$\begin{aligned}\mathbf{D}'(\mathbf{r})/\varepsilon_{0} &= \mathbf{E}'_{\perp}(\mathbf{r}) + \frac{1}{\varepsilon_{0}}\mathbf{P}'_{\perp}(\mathbf{r}) \\ &= \mathbf{E}_{\perp}(\mathbf{r}) \\ &= i\sum_{j}\mathscr{E}_{\omega_{j}}\left(a_{j}\boldsymbol{\varepsilon}_{j}\,\mathrm{e}^{i\mathbf{k}_{j}\cdot\mathbf{r}} - a_{j}^{+}\boldsymbol{\varepsilon}_{j}\,\mathrm{e}^{-i\mathbf{k}_{j}\cdot\mathbf{r}}\right).\end{aligned} \tag{89}$$

$$\begin{aligned}\mathbf{E}'_{\perp}(\mathbf{r}) &= T\mathbf{E}_{\perp}(\mathbf{r})T^{+} \\ &= \sum_{j}\mathscr{E}_{\omega_{j}}\left[i\left(a_{j} + \lambda_{j}\right)\boldsymbol{\varepsilon}_{j}\,\mathrm{e}^{i\mathbf{k}_{j}\cdot\mathbf{r}} + \text{h.c.}\right] \\ &= \mathbf{E}_{\perp}(\mathbf{r}) - \frac{1}{\varepsilon_{0}}\mathbf{P}_{\perp}(\mathbf{r})\end{aligned} \tag{81}$$

$$\mathbf{P}(\mathbf{r}) = \mathbf{d}\,\delta(\mathbf{r}) \tag{82}$$

$$H_{I}' = -\mathbf{d} \cdot \mathbf{D}'(0)/\varepsilon_{0}$$

$$H_{I}' = -\mathbf{d} \cdot \mathbf{E}_{\perp}(0)$$