APPPHYS383 Thursday 7 January 2010

Summary points

Much of the following utilizes supplementary material from *Photons & Atoms: Introduction to Quantum Electrodynamics*, by C. Cohen-Tannoudji, J. Dupont-Roc and G. Grynberg, henceforth referred to as "P&A." Section references are for the 1989 edition.

• The classical nonrelativistic dynamics of a set of charged particles and electromagnetic fields is in principle governed by the standard Lagrangian,

$$L = L_p + L_R + L_I,$$

$$L_p = \sum_{\alpha} \frac{1}{2} m_{\alpha} \dot{\boldsymbol{r}}_{\alpha}^2,$$

$$L_R = \frac{\varepsilon_0}{2} \int d^3 r [\boldsymbol{E}^2(\boldsymbol{r}) - c^2 \boldsymbol{B}^2(\boldsymbol{r})],$$

$$L_I = \sum [q_{\alpha} \dot{\boldsymbol{r}}_{\alpha} \cdot \boldsymbol{A}(\boldsymbol{r}_{\alpha}) - q_{\alpha} U(\boldsymbol{r}_{\alpha})].$$

One can for example derive from *L* both the Maxwell Equations, which describe the dynamics of the fields and the influence on them of charged particle motions, and the Newton-Lorentz equation for particle motion driven by the fields.

• Before performing canonical quantization we need to eliminate any redundant generalized coordinates in the Lagrangian. The first step towards doing this is to replace E(r) and B(r) with

$$E(\mathbf{r}) = -\nabla U(\mathbf{r}) - \dot{A}(\mathbf{r}),$$

$$B(\mathbf{r}) = \nabla \times A(\mathbf{r}).$$

If we take into account the fact that U(r) is algebraically determined by the $\{r_{\alpha}\}$, this leaves us with a Lagrangian $L(\{r_{\alpha}\}, \{\dot{r}_{\alpha}\}, A(r), \dot{A}(r))$.

• In atomic physics it is rare that we work directly in terms of the real-space fields E(r) and B(r) or the real-space vector potential A(r). The kinds of propagating EM fields we can create with lasers and standard optics, and the absorption/emission properties of gas-phase atoms are much more conveniently described in reciprocal space, working with the Fourier transform fields E(k,t), B(k,t), A(k,t) and $\dot{A}(k,t)$. The standard Lagrangian can be rewritten in reciprocal space as

$$L = \sum_{\alpha} \frac{1}{2} m_{\alpha} \dot{r}_{\alpha}^{2} + \int_{+} d^{3}k \,\bar{\mathbf{L}},$$

$$\bar{\mathbf{L}} = \varepsilon_{0} \Big[\left| \dot{A}(\mathbf{k}) + i\mathbf{k}U(\mathbf{k}) \right|^{2} - c^{2} |\mathbf{k} \times A(\mathbf{k})|^{2} \Big] + \big[\mathbf{j}^{*}(\mathbf{k}) \cdot A(\mathbf{k}) + \mathbf{j}(\mathbf{k}) \cdot A^{*}(\mathbf{k}) - \rho^{*}(\mathbf{k})U(\mathbf{k}) - \rho(\mathbf{k})U^{*}(\mathbf{k}) \big].$$

Note that the integral is taken only over a half-space, since the fact that the real-space fields cannot have imaginary components imposes the constraint

 $A_{\varepsilon}(-k) = A_{\varepsilon}^*(k),$

on the vector components of A(k). Working in reciprocal space also facilitates the very convenient electric dipole approximation by separating out the contributions of field components on different spatial scales.

 Having made the transition to reciprocal space it also becomes easier to identify one additional reduction in the number of degrees of freedom. By choosing to work in the Coulomb gauge we can eliminate the longitudinal vector potential:

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

$$E_{\perp}(k) = -\frac{\partial}{\partial t}A_{\perp}(k),$$

$$B_{\perp}(k) = ik \times A_{\perp}(k).$$

Hence we are left with four degrees of freedom for the fields, corresponding to the vector components of $A_{\perp}(k)$ and of $\dot{A}_{\perp}(k)$.

According to the Lagrangian formalism for complex fields [see P&A §II.A.2.f], the conjugate momentum associated with field component A_i(k) is

$$\Pi_j(\boldsymbol{k}) = \left(\frac{\partial L}{\partial \dot{A}_j(\boldsymbol{k})}\right)^*,$$

which for our standard electrodynamic Lagrangian evalutes to

$\prod_j(\boldsymbol{k}) = \varepsilon_0 \dot{A}_j(\boldsymbol{k}).$

According to the usual procedure of canonical quantization (for complex fields, see P&A §II.A.2.g) we thus assign a [q,p]-type commutator,

$$\left[A_{\varepsilon}(\boldsymbol{k}), \prod_{\varepsilon'}^{\dagger}(\boldsymbol{k}')\right] = i\hbar\delta_{\varepsilon\varepsilon'}\delta(\boldsymbol{k}-\boldsymbol{k}'),$$

with all other commutators set to zero.

 In order to reveal the underlying harmonic-oscillator character of the quantized field, it is customary to perform one final change of variables to the so-called normal variables (see below),

$$a(k) = \lambda(k) [-A_{\perp}(k) + i\omega A_{\perp}(k)],$$

where $\omega = c|k|$ and $\lambda(k)$ is an arbitrary normalization constant. If we choose $\lambda(k) = -i\sqrt{\varepsilon_0/2\hbar\omega}$ the resulting commutation relations for the operators corresponding to the quantized normal variables are

$$[a_{\varepsilon}(\boldsymbol{k}), a_{\varepsilon'}^{\dagger}(\boldsymbol{k}')] = \delta_{\varepsilon\varepsilon'} \delta(\boldsymbol{k} - \boldsymbol{k}').$$

The quantized Hamiltonian in the Coulomb gauge can be written

$$H = \sum_{\alpha} \frac{1}{2m_{\alpha}} [\boldsymbol{p}_{\alpha} - q_{\alpha} \boldsymbol{A}(\boldsymbol{r}_{\alpha})]^{2} + \sum_{\alpha} \varepsilon_{\text{Coul}}^{\alpha} + \frac{1}{8\pi\varepsilon_{0}} \sum_{\alpha\neq\beta} \frac{q_{\alpha}q_{\beta}}{|\boldsymbol{r}_{\alpha} - \boldsymbol{r}_{\beta}|} + \sum_{i} \hbar\omega_{i} \left(a_{i}^{\dagger}a_{i} + \frac{1}{2}\right),$$

where the summation on *i* runs over all wave vectors and polarizations. We thus find that the observables of the quantized electromagnetic field correspond to the operator algebra of an infinite set of uncoupled harmonic oscillators.

- [from A&P §II.C.5] It should be noted that this approach of applying canonical quantization to the classical electrodynamic Lagrangian results in a theory that correctly describes atomic interactions with optical/rf electromagnetic fields, but does not correctly describe interactions with high frequency modes having $hv \gtrsim mc^2$ (in which there can be processes such as creation of electron-positron pairs, *et cetera*). Obviously the treatment of the particle motions is non-relativistic, but note that since the standard Lagrangian reproduces the Maxwell Equations the fields themselves are relativistically invariant. By working in the Coulomb gauge we sacrifice the elegant formalism in which the vector and scalar potentials are taken as components of a covariant four-vector, but we gain true independence of the dynamic variables which enables us to apply a simple procedure of canonical quantization.
- Finally in the electric dipole approximation we apply the unitary transformation $G' = TGT^{\dagger}$ to all operators, with

$$T = \exp\left[-\frac{i}{\hbar}d \cdot A_{\perp}(0)\right]$$
$$d = \sum_{\alpha} q_{\alpha}r_{\alpha}.$$

It is assumed that the charged particles are located close to the origin, and are globally neutral. This leads to a modified electrodynamic Hamiltonian

$$H' = \sum_{\alpha} \frac{p_{\alpha}^2}{2m_{\alpha}} + \sum_{\alpha} \varepsilon_{\text{Coul}}^{\alpha} + \frac{1}{8\pi\varepsilon_0} \sum_{\alpha\neq\beta} \frac{q_{\alpha}q_{\beta}}{|r_{\alpha} - r_{\beta}|} + \sum_{i} \hbar\omega_i \left(a_i^{\dagger}a_i + \frac{1}{2}\right) - d \cdot E_{\perp}(0).$$

Note that here the first sum on the RHS represents the kinetic energy of the atom, and that $E_{\perp}(0)$ should be replaced by $E_{\perp}(R)$ in scenarios where the atom can move significantly from the origin (R is the center of mass position of the atom). Note that in experiments with cold atoms the $d \cdot E_{\perp}(R)$ coupling can give rise to entanglement between atomic internal (electronic) and external (center-of-mass motional) degrees of freedom.

Disscussion point: normal variables in the classical model

Since the 'normal variables' assume such a central role in the quantized theory (turning into annihilation and creation operators for the field modes), it is interesting to ask what their significance is in the classical model. We begin by looking at the equations of motion (6.a,b) for the transverse fields,

$$\frac{\partial}{\partial t} \boldsymbol{B}_{\perp}(\boldsymbol{k},t) = -i\boldsymbol{k} \times \boldsymbol{E}_{\perp}(\boldsymbol{k},t),$$
$$\frac{\partial}{\partial t} \boldsymbol{E}_{\perp}(\boldsymbol{k},t) = c^{2}i\boldsymbol{k} \times \boldsymbol{B}_{\perp}(\boldsymbol{k},t) - \frac{1}{\varepsilon_{0}}\boldsymbol{j}_{\perp}(\boldsymbol{k},t).$$

If we fix k and choose coordinate axes such that k is parallel to \hat{z} , we can rewrite

$$\boldsymbol{k} \times \boldsymbol{E}_{\perp}(\boldsymbol{k},t) \to k\,\hat{\boldsymbol{z}} \times (E_x\,\hat{\boldsymbol{x}} + E_y\,\hat{\boldsymbol{y}}) = kE_x\,\hat{\boldsymbol{y}} - kE_y\,\hat{\boldsymbol{x}},$$

$$\boldsymbol{k} \times \boldsymbol{B}_{\perp}(\boldsymbol{k},t) \to k \, \hat{\boldsymbol{z}} \times (B_x \, \hat{\boldsymbol{x}} + B_y \, \hat{\boldsymbol{y}}) = k B_x \, \hat{\boldsymbol{y}} - k B_y \, \hat{\boldsymbol{x}},$$

For fixed k we can rewrite these

$$\frac{d}{dt} \begin{bmatrix} B_x \\ B_y \\ E_x \\ E_y \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & ik \\ 0 & 0 & -ik & 0 \\ 0 & -c^2ik & 0 & 0 \\ c^2ik & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} B_x \\ B_y \\ E_x \\ E_y \end{bmatrix} - \frac{1}{\varepsilon_0} \begin{bmatrix} 0 \\ 0 \\ j_x \\ j_y \end{bmatrix}$$

For such a linear dynamical system we know that the time evolution is simplest when viewed in terms of the eigenvectors of the coefficient matrix

$$A = \begin{bmatrix} 0 & 0 & 0 & ik \\ 0 & 0 & -ik & 0 \\ 0 & -c^2 ik & 0 & 0 \\ c^2 ik & 0 & 0 & 0 \end{bmatrix}$$

We can rewrite this in a Jordan canonical form,

$$A = \begin{bmatrix} 0 & -\frac{1}{2c} & 0 & \frac{1}{2c} \\ \frac{1}{2c} & 0 & -\frac{1}{2c} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} -ick & 0 & 0 & 0 \\ 0 & -ick & 0 & 0 \\ 0 & 0 & ick & 0 \\ 0 & 0 & 0 & ick \end{bmatrix} \begin{bmatrix} 0 & c & 1 & 0 \\ -c & 0 & 0 & 1 \\ 0 & -c & 1 & 0 \\ c & 0 & 0 & 1 \end{bmatrix},$$

from which it follows that we should consider the modified set of variables

$$\begin{bmatrix} 0 & c & 1 & 0 \\ -c & 0 & 0 & 1 \\ 0 & -c & 1 & 0 \\ c & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} B_x \\ B_y \\ E_x \\ E_y \end{bmatrix} = \begin{bmatrix} E_x + cB_y \\ E_y - cB_x \\ E_x - cB_y \\ E_y + cB_x \end{bmatrix}$$

In terms of these the dynamical equations are

$$\frac{d}{dt} \begin{bmatrix}
E_x + cB_y \\
E_y - cB_x \\
E_x - cB_y \\
E_y + cB_x
\end{bmatrix} =
\begin{bmatrix}
-ick & 0 & 0 & 0 \\
0 & -ick & 0 & 0 \\
0 & 0 & ick & 0 \\
0 & 0 & 0 & ick
\end{bmatrix}
\begin{bmatrix}
E_x + cB_y \\
E_y - cB_x \\
E_x - cB_y \\
E_y + cB_x
\end{bmatrix} - \frac{1}{\varepsilon_0} \begin{bmatrix}
0 & c & 1 & 0 \\
-c & 0 & 0 & 1 \\
0 & -c & 1 & 0 \\
c & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
j_x \\
j_y
\end{bmatrix}$$

$$= \begin{bmatrix}
-ick & 0 & 0 & 0 \\
0 & -ick & 0 & 0 \\
0 & 0 & ick & 0 \\
0 & 0 & ick & 0 \\
0 & 0 & 0 & ick
\end{bmatrix}
\begin{bmatrix}
E_x + cB_y \\
E_y - cB_x \\
E_y -$$

Looking at the 'normal variables' as given in the Appendix,

$$\boldsymbol{\alpha}(k\hat{\boldsymbol{z}},t) = \lambda(k) \{ \boldsymbol{E}_{\perp}(\boldsymbol{k},t) - c\hat{\boldsymbol{z}} \times \boldsymbol{B}(\boldsymbol{k},t) \},\\ \boldsymbol{\alpha}_{x}(k\hat{\boldsymbol{z}},t) = \lambda(k) \{ \boldsymbol{E}_{x}(\boldsymbol{k},t) + c\boldsymbol{B}_{y}(\boldsymbol{k},t) \},\\ \boldsymbol{\alpha}_{y}(k\hat{\boldsymbol{z}},t) = \lambda(k) \{ \boldsymbol{E}_{y}(\boldsymbol{k},t) - c\boldsymbol{B}_{x}(\boldsymbol{k},t) \},$$

we recognize that α_x and α_y are simply proportional to the coordinates that we obtain by diagonalizing *A*. If we choose

$$\lambda(k) = -i\sqrt{\varepsilon_0/2\hbar\omega}, \quad \omega = c|\mathbf{k}|$$

as suggested, we see that our equations of motion for the normal variables are simply

$$\dot{\alpha}_x = -ick\,\alpha_x + \frac{i}{\sqrt{2\varepsilon_0\hbar\omega}}j_x,$$
$$\dot{\alpha}_y = -ick\,\alpha_y + \frac{i}{\sqrt{2\varepsilon_0\hbar\omega}}j_y.$$

Hence, in the absence of sources, α_x and α_y undergo simple harmonic oscillations. It can be shown [P&A §I.C.2] that the additional variables

$$\beta_x(k\hat{z},t) \equiv \lambda(k) \{ E_x(k,t) - cB_y(k,t) \}, \beta_y(k\hat{z},t) = \lambda(k) \{ E_y(k,t) + cB_x(k,t) \},$$

are in fact fixed as

$$\boldsymbol{\beta}(\boldsymbol{k},t) = -\boldsymbol{\alpha}^*(\boldsymbol{k},t),$$

because of the constraint that the real-space fields E_{\perp} and **B** cannot have imaginary components.

Discussion point: time-dependent unitary transformations

Before Equation (75) it is noted that $H' = THT^{\dagger}$ because the transformation *T* is time-independent. Sometimes in switching to the interaction picture we will need to use time-dependent transformations, but it is easy to derive the necessary modifications. Consider a general unitary transformation acting on the entire state space,

$$|\Psi'(t)\rangle \equiv U|\Psi(t)\rangle$$

We can start from the Schrödinger Equation

$$\hbar rac{d}{dt} |\Psi(t)
angle = H |\Psi(t)
angle = H U^{-1} |\Psi'(t)
angle$$

and simply apply the chain rule on the left-hand side to yield

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = i\hbar\frac{d}{dt}(U^{-1}|\Psi'(t)\rangle) = i\hbar\left(\frac{dU^{-1}}{dt}|\Psi'(t)\rangle + U^{-1}\frac{d}{dt}|\Psi'(t)\rangle\right)$$
$$i\hbar U^{-1}\frac{d}{dt}|\Psi'(t)\rangle = i\hbar\frac{d}{dt}|\Psi(t)\rangle - i\hbar\frac{dU^{-1}}{dt}|\Psi'(t)\rangle.$$

Hence, combining the two expressions and multiplying through from the left by U, we obtain

$$i\hbar \frac{d}{dt} |\Psi'(t)\rangle = \left(UHU^{-1} - i\hbar U \frac{dU^{-1}}{dt}\right) |\Psi'(t)\rangle$$
$$\equiv H' |\Psi'(t)\rangle.$$

Discussion point: unitary transformations of annihilation operators

In Equation (67) it is noted that for a displacement operator

$$T(\alpha_j) = \exp\left[\alpha_j^* a_j - \alpha_j a_j^{\dagger}\right]$$

where α_i here represents the complex amplitude of a coherent state, we have the identity

$$T(\alpha_j) a_j T^{\dagger}(\alpha_j) = a_j + \alpha_j.$$

In case you aren't familiar with this type of computation, which arises frequently in atomic physics, we note that a wide range of such results can be obtained using various forms of the Campbell-Baker-Haussdorff formula. One such form reads

$$e^{X}Ye^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \cdots,$$

which in this case yields

$$Y = a_j, \quad X = \alpha_j^* a_j - \alpha_j a_j^{\dagger}, \quad [X, Y] = -\alpha_j \left[a_j^{\dagger}, a_j \right] = \alpha_j, \quad [X, [X, Y]] = 0,$$

$$e^X Y e^{-X} = a_j + \alpha_j.$$

Another useful form is

 $\exp(\lambda A)B\exp(-\lambda A) = \exp(\lambda\gamma)B, \quad [A,B] = \gamma B,$

which can be used to compute the results of unitary transformations such as

$$\exp(i\omega ta^{\dagger}a)a\exp(-i\omega ta^{\dagger}a) = \exp(-i\omega t)a.$$

Literature search assignment

For next Tuesday, find a journal article that discusses the significance of corrections to the electric dipole approximation in some aspect of atomic physics. Please send me the journal reference by Monday, and come to class prepared to say a few words about the article.

Discussion problems for Tuesday

By tomorrow (Friday) afternoon, I'll post a few problems for discussion next week.