6: Quantization of the EM-field; preliminaries

Classical variables $\vec{E}, \vec{B}$
$\rightarrow$ Q.M. operators $\hat{\vec{E}}, \hat{\vec{B}}$

Plan:
1. Formulate the equations in a convenient form
2. Repeat quantum harm. osc.

} today

3. Formulate EM-Hamiltonian as a QM-HO
4. Formulate the light-atom Hamiltonian

} Next two lectures

Starting point is Maxwell's equations

$$\begin{cases} \nabla \times \vec{E} = -\dfrac{\partial \vec{B}}{\partial t} \\ \dfrac{1}{\mu_0} \nabla \times \vec{B} = \varepsilon_0 \dfrac{\partial \vec{E}}{\partial t} + \vec{J} \\ \varepsilon_0 \nabla \cdot \vec{E} = \sigma \\ \nabla \cdot \vec{B} = 0 \end{cases}$$

where $\vec{E} = \vec{E}(\vec{r}, t)$ and same for $\vec{B}, \vec{J}, \sigma$
- $\sigma(\vec{r}, t)$ charge density
- $\vec{J}(\vec{r}, t)$ current density

One set of $\vec{B}, \vec{E}$ describes a field.
Inclusion of $\vec{J}, \sigma$ means interaction with matter.

M.E.4 $\Rightarrow$ $\boxed{\vec{B} = \nabla \times \vec{A}}$

def. vector potential!

M.E.1 $\Rightarrow$ $\boxed{\nabla\phi = -\vec{E} - \frac{\partial \vec{A}}{\partial t}}$ def. scalar potential.

M.E.2 $\Rightarrow$ $\nabla \times (\nabla \times \vec{A}) - \varepsilon_0 \mu_0 \frac{\partial \vec{E}}{\partial t} = \mu_0 \vec{J}$

$$\boxed{\nabla(\nabla \cdot \vec{A}) - \nabla^2 \vec{A} + \frac{1}{c^2}\frac{\partial}{\partial t}\nabla\phi + \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = \mu_0 \vec{J}}$$

$$\left(c^2 = \frac{1}{\varepsilon_0 \mu_0}\right)$$

M.E.3 $\Rightarrow$ $\boxed{-\varepsilon_0 \nabla^2 \phi - \varepsilon_0 \nabla \cdot \frac{\partial \vec{A}}{\partial t} = \sigma}$

These are the equations we are going to work with.

- Gauge invariance:

The M.E. (& hence the physics) is left unchanged if we take any function $\chi(\vec{r}, t)$ and replace $\vec{A}', \phi'$ by $\vec{A}, \phi$, where the new potentials are defined by

$$\boxed{\begin{aligned} \vec{A} &= \vec{A}' - \nabla\chi \\ \phi &= \phi' + \frac{\partial \chi}{\partial t} \end{aligned}}$$

Best suited for our problem is the

Coulomb gauge:

Choose $\vec{A}, \phi$ such that

$$\boxed{\nabla\cdot\vec{A} = 0}$$

(I.e. if we have $\vec{A}'$ such that $\nabla\cdot\vec{A}' \neq 0$, then define χ so that $\nabla^2\chi = \nabla\cdot\vec{A}'$)

In the Coulomb gauge:

ME 2 $$-\nabla^2\vec{A} + \frac{1}{c^2}\frac{\partial}{\partial t}\nabla\phi + \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = \mu_0\vec{J}$$

ME 3 $$-\nabla^2\phi = \frac{\sigma}{\varepsilon_0}$$

Now some vector calculus

A vector field $\vec{W}(\vec{r})$ is called <u>longitudinal</u> or curl-free if

$$\nabla\times\vec{W} = 0$$

It is called <u>transverse</u> or divergence-free if

$$\nabla\cdot\vec{W} = 0$$

Theorem: Any vector field $\vec{V}(\vec{r})$ can be written as a <u>sum</u>

$$\vec{V}(\vec{r}) = \vec{V}_L(\vec{r}) + \vec{V}_T(\vec{r})$$

where $\vec{V}_L$ is long. and $\vec{V}_T$ is transv.

Proof of theorem: By construction.
Calculate the Fourier transform

$$\vec{V}(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{r}\, e^{-i\vec{k}\cdot\vec{r}}\, \vec{V}(\vec{r})$$

(Optional material!)

Define $\vec{V}_L(\vec{k}) = \frac{\vec{k}}{|\vec{k}|^2}\, \vec{k}\cdot\vec{V}(\vec{k})$

or in terms of components $i, j = x, y, z$:

$$V_{iL}(\vec{k}) = \frac{k_i}{|\vec{k}|^2} \sum_j k_j V_j(\vec{k})$$

and define $\vec{V}_T(\vec{k}) = \vec{V}(\vec{k}) - \vec{V}_L(\vec{k})$

Then Fourier transform back:

$$\vec{V}_{L,T}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{k}\, e^{i\vec{k}\cdot\vec{r}}\, \vec{V}_{L,T}(\vec{k})$$

By definition, $\vec{V}(\vec{r}) = \vec{V}_L(\vec{r}) + \vec{V}_T(\vec{r})$

and you can check that

$$\begin{cases} \nabla\times\vec{V}_L(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{k}\, e^{i\vec{k}\cdot\vec{r}}\, \vec{k}\times\vec{V}_L(\vec{k}) = 0 \\ \nabla\cdot\vec{V}_T(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int d^3\vec{k}\, e^{i\vec{k}\cdot\vec{r}}\, \vec{k}\cdot\vec{V}_T(\vec{k}) = 0 \end{cases}$$

Q.E.D.

So we have $\vec{A} = \vec{A}_L + \vec{A}_T$ in general.

Note that

$$\vec{B} = \vec{\nabla}\times\vec{A} = \vec{\nabla}\times\vec{A}_T$$

In Coulomb gauge, $\vec{A}$ is transverse: $\vec{A} = \vec{A}_T$ & $\vec{A}_L = 0$

Also observe: $\nabla\times\nabla\phi = 0$, so $\nabla\phi$ is longitudinal.

Then M.E.2 can be broken up into L & T parts

$$(ME2)_L: \quad \frac{1}{c^2}\frac{\partial}{\partial t}\nabla\phi = \mu_0 \vec{J}_L$$

$$(ME2)_T = -\nabla^2\vec{A} + \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = \mu_0\vec{J}_T$$

(in Coulomb gauge)

Note also $\left.\begin{aligned} \vec{E}_T &= -\frac{\partial\vec{A}}{\partial t} \\ \vec{E}_L &= -\nabla\phi \end{aligned}\right\}$ in Coulomb gauge

$\left.\begin{aligned} \vec{B}_T &= \nabla\times\vec{A} \\ \vec{B}_L &= 0 \end{aligned}\right\}$ always

One may say that:

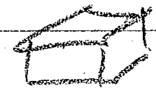
$$\left\{\begin{array}{l} \text{longitudinal fields} \leftrightarrow \text{electrostatics} \\ \text{transverse fields} \leftrightarrow \text{Radiation} \end{array}\right.$$

Free field

First deal with free field – no matter.

$$\vec{J}_T = 0$$

$$\Rightarrow \quad -\nabla^2 \vec{A} + \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = 0$$

"Box" geometry $L \times L \times L$ 

with periodic boundary conditions $\vec{A}(x,y,z) = \vec{A}(x+L,y,z)$
$= \vec{A}(x,y+L,z)$
$= \vec{A}(x,y,z+L)$

Solutions

$$\vec{A}_{\vec{k}\lambda}(\vec{r},t) = \vec{e}_{\vec{k}\lambda} A_{\vec{k}\lambda}(\vec{r},t)$$

where (scalar!)

$$A_{\vec{k}\lambda}(\vec{r},t) = A_{\vec{k}\lambda}\, e^{i(-\omega_k t + \vec{k}\cdot\vec{r})} + A^*_{\vec{k}\lambda}\, e^{i(\omega_k t - \vec{k}\cdot\vec{r})}$$

and $\vec{e}_{k\lambda}$ is a unit vector for the direction of $\vec{A}$

Coulomb gauge: $\nabla\cdot\vec{A} = 0 \Rightarrow \vec{k}\cdot\vec{e}_{\vec{k}\lambda} = 0$

$\Rightarrow$ two linearly independent directions $\lambda = 1,2$

$$\vec{e}_{\vec{k}1}\cdot\vec{e}_{\vec{k}2} = 0 \quad \text{or}$$

$$\vec{e}_{\vec{k}\lambda}\cdot\vec{e}_{\vec{k}\lambda'} = \delta_{\lambda\lambda'}$$

where Kronecker delta: $\delta_{ij} = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i\neq j \end{cases}$

Finally, $\omega_k = ck$.

General solution

$$\vec{A}(\vec{r},t) = \sum_{\vec{k}} \sum_{\lambda=1}^{2} \hat{e}_{\vec{k}\lambda} A_{\vec{k}\lambda}(\vec{r},t)$$

Calculate

$$\vec{E}_T(\vec{r},t) = \sum_{\vec{k}} \sum_{\lambda=1}^{2} \hat{e}_{\vec{k}\lambda} E_{\vec{k}\lambda}(\vec{r},t) \qquad \text{transverse part}$$

$$E_{\vec{k}\lambda}(\vec{r},t) = i\omega_k \left\{ A_{\vec{k}\lambda} e^{-i\omega_k t + i\vec{k}\cdot\vec{r}} - A^*_{\vec{k}\lambda} e^{i\omega_k t - i\vec{k}\cdot\vec{r}} \right\}$$

$$\vec{B}(\vec{r},t) = \sum_{\vec{k}} \sum_{\lambda=1}^{2} \frac{\vec{k}\times\vec{e}_{\vec{k}\lambda}}{k} B_{\vec{k}\lambda}(\vec{r},t)$$

$$B_{\vec{k}\lambda}(\vec{r}t) = ik \left\{ A_{\vec{k}\lambda} e^{-i\omega_k t + i\vec{k}\cdot\vec{r}} - A^*_{\vec{k}\lambda} e^{i\omega_k t - i\vec{k}\cdot\vec{r}} \right\}$$

Total energy of the radiation field:

$$\mathcal{E}_R = \frac{1}{2} \int d^3\vec{r} \left[\varepsilon_0 |\vec{E}(\vec{r},t)|^2 + \frac{1}{\mu_0} |\vec{B}(\vec{r},t)|^2 \right]$$

$$= \ldots$$

$$= \frac{1}{2} \sum_{\vec{k}\lambda} \mathcal{E}_{\vec{k}\lambda}$$

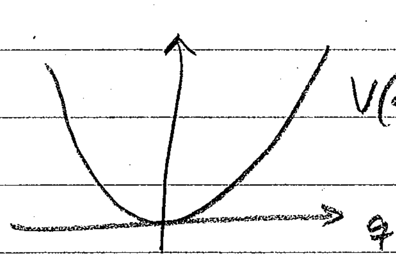
where

$$\mathcal{E}_{\vec{k}\lambda} = \varepsilon_0 V \omega_k^2 \left(A_{k\lambda} A^*_{k\lambda} + A^*_{k\lambda} A_{k\lambda} \right)$$

As long as $A_{k\lambda}$ are classical variables, they commute and we could just write $2|A_{k\lambda}|^2$
But we anticipate quantization!

Repeat: the harmonic oscillator in q.m.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{q}^2$$



$V(q) = \frac{1}{2} m\omega^2 q^2$

where

$$[\hat{q}, \hat{p}] = i\hbar$$

Go to new operators by

$$\boxed{\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}\,\hat{q} + \frac{i}{\sqrt{\hbar m\omega}}\,\hat{p}\right) \\ \hat{a}^+ &= \frac{1}{\sqrt{2}}\left(\qquad - \qquad \right) \end{aligned}}$$

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}\,(\hat{a}^+ + \hat{a})$$

$$\hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}\,(\hat{a}^+ - \hat{a})$$

Then

$$[\hat{a}, \hat{a}^+] = \frac{1}{2}\left[\sqrt{\frac{m\omega}{\hbar}}\,\hat{q} + \frac{i}{\sqrt{m\hbar\omega}}\,\hat{p},\ \sqrt{\frac{m\omega}{\hbar}}\,\hat{q} - \frac{i}{\sqrt{m\hbar\omega}}\,\hat{p}\right]$$

$$= \frac{1}{2}\left(\frac{1}{\hbar}(-i)\,[\hat{q}, \hat{p}] + \frac{i}{\hbar}\,[\hat{p}, \hat{q}]\right)$$

$$= 1$$

$$\hat{H} = -\frac{1}{2m}\left(\frac{m\hbar\omega}{2}\right)(\hat{a}^+ - \hat{a})^2 + \frac{1}{2} m\omega^2 \frac{\hbar}{2m\omega}(\hat{a}^+ + \hat{a})^2$$

$$= \frac{\hbar\omega}{4}\left[(\hat{a}^+ + \hat{a})^2 - (\hat{a}^+ - \hat{a})^2\right]$$

$$= \frac{\hbar\omega}{2}\left(\hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right)$$

$$= \boxed{\hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)}$$

Eigenvalue equation:

Which states are eigenstates of $\hat{H}$?

Consider an eigenstate which we choose to call $|n\rangle$:

$$\hat{H}|n\rangle = \hbar\omega\left(\hat{a}^{+}\hat{a} + \tfrac{1}{2}\right)|n\rangle = E_n|n\rangle$$

Multiply from left by $\hat{a}^{+}$

$$\hbar\omega\left(\underbrace{\hat{a}^{+}\hat{a}^{+}\hat{a}}_{=\hat{a}^{+}(\hat{a}\hat{a}^{+}-1)\ \text{by commutation relation}} + \tfrac{1}{2}\hat{a}^{+}\right)|n\rangle = E_n\hat{a}^{+}|n\rangle$$

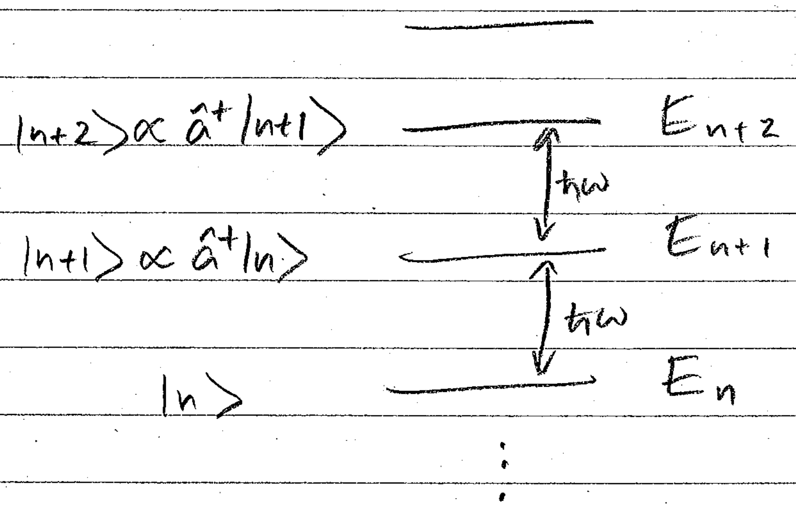
$$\Rightarrow \hbar\omega\left(\hat{a}^{+}\hat{a}\hat{a}^{+} - \hat{a}^{+} + \tfrac{1}{2}\hat{a}^{+}\right)|n\rangle = E_n\hat{a}^{+}|n\rangle$$

$$\underbrace{\hbar\omega\left(\hat{a}^{+}\hat{a} + \tfrac{1}{2}\right)}_{=\hat{H}}\hat{a}^{+}|n\rangle = \left(E_n + \hbar\omega\right)\hat{a}^{+}|n\rangle$$

$\therefore$ If $|n\rangle$ is eigenstate with E_n

then $\hat{a}^{+}|n\rangle$ — " — $E_n + \hbar\omega$

$\Rightarrow$ we have a discrete spectrum



(Normalization will fix proportionality.)

- Because $\hat{H}$ is positive definite (the sum of the squares of two Hermitian operators) then we know all $E_n \geq 0$

$\Rightarrow$ there must be a <u>lowest</u> E_n = a ground state.

- By same algebra as above, have

$$\hat{a}|n\rangle \propto |n-1\rangle \; ; \; \hat{H}|n-1\rangle = (E_n - \hbar\omega)|n-1\rangle$$

Then for the ground state $|0\rangle$:

<u>Must</u> have

$$\hat{a}|0\rangle = 0$$

otherwise there exists a state with <u>lower</u> energy.

Compute:

$$\hat{H}|0\rangle = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right)|0\rangle$$

$$= \hbar\omega\, \hat{a}^\dagger \underbrace{\left(\hat{a}|0\rangle\right)}_{=0 \text{ by assumption!}} + \tfrac{1}{2}\hbar\omega|0\rangle$$

$$= \tfrac{1}{2}\hbar\omega|0\rangle.$$

$$\therefore \begin{cases} E_0 = \tfrac{1}{2}\hbar\omega \\ E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2, \ldots \end{cases}$$

Def. <u>number operator</u> $\hat{n} = \hat{a}^\dagger\hat{a}$

Then $\hat{n}|n\rangle = \left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)|n\rangle = n|n\rangle$

$\hat{n}$ counts the "<u>degree</u> of <u>excitation</u>" of the state.

Normalization: $\langle n|n\rangle = 1$

Assume $\hat{a}|n\rangle = C_n|n-1\rangle$, C_n complex number

Then

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = \langle n-1|n-1\rangle|C_n|^2 = |C_n|^2$$
$$= \langle n|\hat{n}|n\rangle = n$$
$$\Rightarrow \quad C_n = \sqrt{n} \quad \text{(can be chosen real \& positive)}$$

so
$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$$
$$\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

Note: $|n\rangle$ are "number states":
eigenstates of $\hat{n}$ and $\hat{H}$.
More general states can be constructed
$$|\psi\rangle = \sum_{n=0}^{\infty} b_n|n\rangle$$
will not be eigenstates of $\hat{H}$.