MIT Department of Chemistry 5.74, Spring 2004: Introductory Quantum Mechanics II Instructor: Prof. Andrei Tokmakoff

Non-Lecture

Review of Free Electromagnetic Field

Maxwell's Equations (SI):

(1)
$$\overline{\nabla} \cdot \overline{B} = 0$$

(2)
$$\overline{\nabla} \cdot \overline{E} = \rho / \in_0$$

(3)
$$\overline{\nabla} \times \overline{E} = -\frac{\partial \overline{B}}{\partial t}$$

(4)
$$\overline{\nabla} \times \overline{B} = \mu_0 \overline{J} + \epsilon_0 \ \mu_0 \frac{\partial \overline{E}}{\partial t}$$

 \overline{E} : electric field; \overline{B} : magnetic field; \overline{J} : current density; ρ : charge density; ϵ_0 : electrical permittivity; μ_0 : magnetic permittivity

We are interested in describing \overline{E} and \overline{B} in terms of a scalar and vector <u>potential</u>. This is required for our interaction Hamiltonian.

<u>Generally</u>: A <u>vector</u> field \overline{F} assigns a vector to each point in space, and:

(5)
$$\overline{\nabla} \cdot \overline{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$$
 is a scalar

For a scalar field ϕ

(6)
$$\nabla \phi = \frac{\partial \phi}{\partial x} \hat{x} + \frac{\partial \phi}{\partial y} \hat{y} + \frac{\partial \phi}{\partial z} \hat{z}$$
 is a vector

where $\hat{x}^2 + \hat{y}^2 + \hat{z}^2 = \hat{r}^2$ unit vector

Also:

(7)
$$\overline{\nabla} \times \overline{F} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix}$$

Some useful identities from vector calculus are:

(8)
$$\overline{\nabla} \cdot \left(\overline{\nabla} \times \overline{F}\right) = 0$$

$$(9) \qquad \nabla \times (\nabla \phi) = 0$$

(10)
$$\nabla \times \left(\overline{\nabla} \times \overline{F} \right) = \overline{\nabla} \left(\overline{\nabla} \cdot \overline{F} \right) - \overline{\nabla}^2 \overline{F}$$

We now introduce a vector potential $\overline{A}(\overline{r},t)$ and a scalar potential $\varphi(\overline{r},t)$, which we will relate to \overline{E} and \overline{B}

Since $\overline{\nabla} \cdot \overline{B} = 0$ and $\overline{\nabla} (\overline{\nabla} \times \overline{A}) = 0$:

(11)
$$\overline{B} = \overline{\nabla} \times \overline{A}$$

(12)

Using (3), we have:

$$\overline{\nabla} \times \overline{E} = -\overline{\nabla} \times \frac{\partial \overline{A}}{\partial t}$$
or
$$\overline{\nabla} \times \left[\overline{E} + \frac{\partial \overline{A}}{\partial t}\right] = 0$$

From (9), we see that a scalar product exists with:

(13)
$$\overline{E} + \frac{\partial \overline{A}}{\partial t} = -\overline{\nabla} \varphi(\overline{r}, t)$$

or convention

(14)
$$\overline{E} = \frac{\partial \overline{A}}{\partial t} - \nabla \varphi$$

So we see that the potentials \overline{A} and φ determine the fields \overline{B} and \overline{E} :

(15)
$$\overline{B}(\overline{r},t) = \overline{\nabla} \times \overline{A}(\overline{r},t)$$

(16)
$$\overline{E}(\overline{r},t) = -\overline{\nabla} \varphi(\overline{r},t) - \frac{\partial}{\partial t} \overline{A}(\overline{r},t)$$

We are interested in determining the wave equation for \overline{A} and φ . Using (15) and differentiating (16) and substituting into (4):

(17)
$$\overline{\nabla} \times \left(\overline{\nabla} \times \overline{A}\right) + \epsilon_0 \ \mu_0 \left(\frac{\partial^2 \overline{A}}{\partial t^2} + \overline{\nabla} \frac{\partial \varphi}{\partial t}\right) = \mu_0 \overline{J}$$

Using (10):

(18)
$$\left[-\overline{\nabla}^{2}\overline{A} + \epsilon_{0} \ \mu_{0} \ \frac{\partial^{2}\overline{A}}{\partial t^{2}}\right] + \overline{\nabla}\left(\overline{\nabla}\cdot\overline{A} + \epsilon_{0} \ \mu_{0} \ \frac{\partial\varphi}{\partial t}\right) = \overline{\mu}_{0} \ \overline{J}$$

From (14), we have:

$$\overline{\nabla} \cdot \overline{E} = -\frac{\partial \overline{\nabla} \cdot \overline{A}}{\partial t} - \overline{\nabla}^2 \varphi$$

and using (2):

(19)
$$\frac{-\partial V \cdot A}{\partial t} - \overline{\nabla}^2 \varphi = \rho / \in_0$$

Notice from (15) and (16) that we only need to specify <u>four</u> field components (A_x, A_y, A_z, φ) to determine all <u>six</u> \overline{E} and \overline{B} components. But \overline{E} and \overline{B} do not uniquely determine \overline{A} and φ . So, we can construct \overline{A} and φ in any number of ways without changing \overline{E} and \overline{B} . Notice that if we change \overline{A} by adding $\overline{\nabla}\chi$ where χ is any function of \overline{r} and t, this won't change \overline{B} ($\nabla \times (\nabla \cdot B) = 0$). It will change E by $\left(-\frac{\partial}{\partial t}\overline{\nabla}\chi\right)$, but we can change φ to $\varphi' = \varphi - \frac{\partial\chi}{\partial t}$. Then \overline{E} and \overline{B} will both be unchanged. This property of changing representation (gauge) without changing \overline{E} and \overline{B} is gauge invariance. We can transform between gauges with:

(20)
$$\overline{A'(\bar{r},t)} = \overline{A(\bar{r},t)} + \overline{\nabla} \cdot \chi(\bar{r},t)$$

(21) $\varphi'(\bar{r},t) = \varphi(\bar{r},t) - \frac{\partial}{\partial t} \chi(\bar{r},t)$

$$\overline{gauge}$$
transformation

Up to this point, A' and Q are undetermined. Let's choose a χ such that:

(22)
$$\overline{\nabla} \cdot \overline{A} + \epsilon_0 \ \mu_0 \frac{\partial \varphi}{\partial t} = 0$$
 Lorentz condition

then from (17):

(23)
$$-\nabla^2 \overline{A} + \epsilon_0 \ \mu_0 \frac{\partial^2 \overline{A}}{\partial t^2} = \mu_0 \overline{J}$$

The RHS can be set to zero for no currents.

From (19), we have:

(24)
$$\in_0 \mu_0 \frac{\partial^2 \varphi}{\partial t^2} - \nabla^2 \varphi = \frac{\rho}{\epsilon_0}$$

Eqns. (23) and (24) are wave equations for \overline{A} and φ . Within the Lorentz gauge, we can still arbitrarily add another χ (it must only satisfy 22). If we substitute (20) and (21) into (24), we see:

(25)
$$\nabla^2 \chi - \epsilon_0 \mu_0 \frac{\partial^2 \chi}{\partial t^2} = 0$$

So we can make further choices/constraints on \overline{A} and φ as long as it obeys (25). For a field far from charges and currents, J = 0 and $\rho = 0$.

(26)
$$-\overline{\nabla}^2 \overline{A} + \epsilon_0 \ \mu_0 \frac{\partial^2 \overline{A}}{\partial t^2} = 0$$

(27)
$$-\overline{\nabla}^2 \varphi + \epsilon_0 \ \mu_0 \frac{\partial^2 \varphi}{\partial t^2} = 0$$

We now choose $\varphi = 0$ (Coulomb gauge), and from (22) we see:

(28)
$$\overline{\nabla} \cdot \overline{A} = 0$$

So, the wave equation for our vector potential is:

(29)
$$-\overline{\nabla}^2 \overline{A} + \epsilon_0 \ \mu_0 \frac{\partial^2 \overline{A}}{\partial t^2} = 0$$

The solutions to this equation are plane waves.

(30)
$$\overline{A} = \overline{A}_0 \sin(\omega t - \overline{k} \cdot \overline{r} + \alpha)$$

 α : phase

(31)
$$= \overline{A}_0 \cos(\omega t - \overline{k} \cdot \overline{r} + \alpha')$$

 \overline{k} is the wave vector which points along the direction of propagation and has a magnitude:

(32) $k^2 = \omega^2 \mu_0 \in \omega^2 / c^2$ Since (28) $\overline{\nabla} \cdot \overline{A} = 0$

$$-\overline{k} \cdot \overline{A}_0 \cos(\omega t - \overline{k} \cdot \overline{r} + \alpha) = 0$$
(33) $\therefore \quad \overline{k} \cdot \overline{A}_0 = 0$
 $\overline{k} \perp \overline{A}_0$

 A_0 is the direction of the potential \rightarrow polarization. From (15) and (16), we see that for $\varphi = 0$:

$$\overline{E} = -\frac{\partial \overline{A}}{\partial t} = -\omega \overline{A}_0 \cos(\omega t - \overline{k} \cdot \overline{r} + \alpha)$$

$$\overline{B} = \overline{\nabla} \times \overline{A} = -(\overline{k} \times \overline{A}_0) \cos(\omega t - \overline{k} \cdot \overline{r} + \alpha)$$

 $\therefore \quad \overline{k} \perp \overline{E} \perp \overline{B}$

