# CHAPTER 4: Multipoles, Electrostatics of Macroscopic Media, Dielectrics

## 4.1 Multipole Expansion

In Ch. 3, we developed various methods of expansion to solve the Poisson equation for  $\phi(\mathbf{x})$ , with an emphasis on mathematics.

Here, we continue the subject of electrostatics by taking a closer look at  $\rho(\mathbf{x})$ , with an emphasis on applications. By the method of expansion, we first decompose the RHS of

$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3 x' \left[ \text{Applicable to infinite space} \right]$$
 (1.17)

into multipole fields and thereby express  $\rho(\mathbf{x})$  in multipole moments.

Applying the results to materials, we find that the atomic/molecular dipole moments account for the electrical properties of a dielectric medium. We then show that these properties can be characterized by a single parameter: the dielectric constant.

#### 4.1 Multipole Expansion (continued)

## **Multipole Expansion in Spherical Coordinates:**

$$\frac{1}{|\mathbf{x} - \mathbf{x}'|} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{2l+1} \frac{r_{<}^{l}}{r_{>}^{l+1}} Y_{lm}^{*}(\theta', \varphi') Y_{lm}(\theta, \varphi)$$
(3.70)

For x outside the sphere enclosing  $\rho$ ,  $r_{<} = r'$ ,  $r_{>} = r$ .

$$\Rightarrow \phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3 x'$$

$$= \frac{1}{\varepsilon_0} \sum_{lm} \frac{1}{2l+1} \left[ \int_{\mathcal{V}} Y_{lm}^*(\theta', \varphi') r'^l \rho(\mathbf{x}') d^3 x' \right] \frac{Y_{lm}(\theta, \varphi)}{r^{l+1}}$$

$$\equiv q_{lm} \text{ (multipole moments)}$$

$$(4.2)$$

A conceptural picture of multipole moments:

monopole 
$$(l=0)$$
  $[+]$   $\Rightarrow \phi \propto \frac{1}{r}$  dipole  $(l=1)$   $[+-]$   $\Rightarrow \phi \propto \frac{1}{r^2}$  partial cancellation of monopoles quadrupole  $(l=2)$   $\begin{bmatrix} + & - \\ - & + \end{bmatrix}$   $\Rightarrow \phi \propto \frac{1}{r^3}$  partial cancellation of dipoles

## Multipole Expansion in Cartesian (Rectangular) Coordinates:

Expansion in Cartesian coordinates is more useful for our purposes. We first summarize the formulae needed for the expansion.

Taylor expansion about point x: [see Appendix A]

$$f(\mathbf{x} + \mathbf{a}) = f(\mathbf{x}) + (\mathbf{a} \cdot \nabla)f(\mathbf{x}) + \frac{1}{2}(\mathbf{a} \cdot \nabla)(\mathbf{a} \cdot \nabla)f(\mathbf{x}) + \cdots, \tag{1}$$

where  $\begin{cases} \mathbf{a} \cdot \nabla = a_1 \frac{\partial}{\partial x_1} + a_2 \frac{\partial}{\partial x_2} + a_3 \frac{\partial}{\partial x_3} = \sum_{i=1}^3 a_i \frac{\partial}{\partial x_i} \\ (\mathbf{a} \cdot \nabla)(\mathbf{a} \cdot \nabla) = \sum_i a_i \frac{\partial}{\partial x_i} \sum_j a_j \frac{\partial}{\partial x_j} = \sum_{ij} a_i a_j \frac{\partial^2}{\partial x_i \partial x_j} \end{cases}$ (2a)

and all derivatives are evaluated at x.

Other useful relations:

$$\nabla |\mathbf{x} - \mathbf{x}'|^n = n |\mathbf{x} - \mathbf{x}'|^{n-2} (\mathbf{x} - \mathbf{x}') \qquad \begin{bmatrix} \text{Eq. (1), lecture} \\ \text{notes, Ch. 1} \end{bmatrix}$$
(3a)

$$\frac{\partial}{\partial x_i} |\mathbf{x} - \mathbf{x}'|^n = n |\mathbf{x} - \mathbf{x}'|^{n-2} (x_i - x_i')$$
(3b)

#### 4.1 Multipole Expansion (continued)

Rewrite 
$$\begin{cases} f(\mathbf{x} + \mathbf{a}) = f(\mathbf{x}) + (\mathbf{a} \cdot \nabla)f(\mathbf{x}) + \frac{1}{2}(\mathbf{a} \cdot \nabla)(\mathbf{a} \cdot \nabla)f(\mathbf{x}) + \cdots & (1) \\ (\mathbf{a} \cdot \nabla)(\mathbf{a} \cdot \nabla) = \sum_{i} a_{i} \frac{\partial}{\partial x_{i}} \sum_{j} a_{j} \frac{\partial}{\partial x_{j}} = \sum_{ij} a_{i} a_{j} \frac{\partial^{2}}{\partial x_{i} \partial x_{j}} & (2b) \\ \nabla |\mathbf{x} - \mathbf{x}'|^{n} = n|\mathbf{x} - \mathbf{x}'|^{n-2}(\mathbf{x} - \mathbf{x}') & \mathbf{x}' & (3a) \end{cases}$$

$$\underbrace{\begin{aligned} \text{Use (1). Let } f(\mathbf{x}) &= 1/|\mathbf{x}| = 1/r \text{ and } \mathbf{a} &= -\mathbf{x}'. \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{j}' \frac{\partial^{2}}{\partial x_{i} \partial x_{j}} \frac{1}{r} + \cdots \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{j}' \frac{\partial^{2}}{\partial x_{i}} = x_{j} \frac{3x_{i}}{r^{5}} - \frac{\delta_{ij}}{r^{3}} \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x}' & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{j}' x_{i}' x_{j} - \frac{1}{2} \sum_{ij} x_{i}' x_{j}' \delta_{ij} \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x}' & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{j}' x_{i}' x_{j} - \frac{1}{2} \sum_{ij} x_{i}' x_{j}' \delta_{ij} \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{j}' x_{i}' x_{j} - \frac{1}{2} \sum_{ij} x_{i}' x_{j}' \delta_{ij} + \cdots \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{j}' x_{i}' x_{j}' x_{i}' x_{j} - \frac{1}{2} \sum_{ij} x_{i}' x_{j}' \delta_{ij} + \cdots \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{i}' x_{j}' x_{i}' x_{j}' x_{i}' x_{j}' - \frac{1}{2} \sum_{ij} x_{i}' x_{i}' x_{j}' \delta_{ij} + \cdots \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{i}' x_{j}' x_{i}' x_{j}' - \frac{1}{2} \sum_{ij} x_{i}' x_{i}' x_{j}' \delta_{ij}' + \cdots \end{aligned}}_{\mathbf{x} - \mathbf{x}'} & \underbrace{\begin{aligned} \text{Use (2b), (3a)} \\ \mathbf{x} - \mathbf{x} & = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^{3}} + \frac{1}{2} \sum_{ij} x_{i}' x_{i}' x_{i}' x_{i}' x_{i}' x_{i}' - \frac{1}{2} \sum_{ij} x_{i}' x_{i}'$$

See (3.70), (3.148), & (3.164) for other expressions of  $\frac{1}{|\mathbf{x}-\mathbf{x}'|}$  in  $\infty$  space.

#### 4.1 Multipole Expansion (continued)

Multipole moments with respect to (w.r.t.)  $\mathbf{x} = 0$ :

Rewrite 
$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^3} + \frac{1}{2r^5} \sum_{ij} x_i x_j \left(3x_i' x_j' - r'^2 \delta_{ij}\right) + \cdots$$
(4)
$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} d^3 x' \xrightarrow{\text{monopole moment}} \frac{\text{dipole moment}}{\text{moment}}$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{\int \rho(\mathbf{x}') d^3 x'}{r} + \frac{\mathbf{x} \cdot \int \mathbf{x}' \rho(\mathbf{x}') d^3 x'}{r^3} + \frac{\rho(\mathbf{x}')}{r^3} \frac{\rho(\mathbf{x}')}{\text{quadrupole moment}} \right]$$

$$+ \frac{1}{2r^5} \sum_{ij} x_i x_j \int (3x_i' x_j' - r'^2 \delta_{ij}) \rho(\mathbf{x}') d^3 x' + \cdots$$

$$= \frac{1}{4\pi\varepsilon_0} \left( \frac{q}{r} + \frac{\mathbf{p} \cdot \mathbf{x}}{r^3} + \frac{1}{2r^5} \sum_{ij} Q_{ij} x_i x_j + \cdots \right)$$

$$Note:$$
(4.10)

- 1. q,  $\mathbf{p}$ ,  $Q_{ij}$ ,  $\cdots$  are *constants* characterizing the charge distribution  $\rho(\mathbf{x})$ .
- 2.  $\mathbf{p}$ ,  $Q_{ij}$ ,  $\cdots$  are defined w.r.t. a <u>reference point</u> [it is  $\mathbf{x} = 0$  in (4.10)].

Question: What are the merit and limitation of (4.10)? See next page.

#### **4.1 Multipole Expansion** (continued)

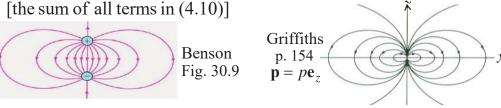
Example: For point charges  $\pm e$  separated by distance d as in the fig., we have  $q = \int \rho(\mathbf{x}')d^3x' = 0$ ,  $\mathbf{p} = \int \mathbf{x}' \rho(\mathbf{x}')d^3x' = ed\mathbf{e}_z$ 

and 
$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3x'$$

$$= \frac{1}{4\pi\varepsilon_0} \left( \frac{\mathcal{A}}{r} + \frac{\mathbf{p} \cdot \mathbf{x}}{r^3} + \frac{1}{2r^5} \sum_{ij} Q_{ij} x_i x_j + \cdots \right) \qquad d \downarrow -e \qquad (4.10)$$

Exact **E** of point charges  $\pm e$  [the sum of all terms in (4.10)]

**E** of the dipole term in (4.10)



Note: A pair of  $\pm e$  consists of all multipole moments (not just  $\mathbf{p}$ ). Merit of (4.10): In the far zone,  $\mathbf{E}(\text{dipole})$  accurately gives  $\mathbf{E}(\text{exact})$ . Limitation: In the near zone, all terms are needed to give  $\mathbf{E}(\text{exact})$ . Amazingly, each term diverges as  $r \to 0$ , but their sum diverges at  $\pm e$ .

6

*Multipole moments with respect to*  $\mathbf{x} = \mathbf{x}_0$ :

Values of  $\mathbf{p}$ ,  $Q_{ij}$ ,...depend on the choice of the reference point (exception noted in the exercise below), but the sum of all multipole fileds gives the same  $\phi(\mathbf{x})$ . It is thus desirable to choose a reference point to minimize higher moments so that the lowest moment can give a good approximation of the exact  $\phi(\mathbf{x})$ .

We may convert the reference point from  $\mathbf{x} = 0$  in (4.10) to  $\mathbf{x} = \mathbf{x}_0$ by using  $\frac{1}{|\mathbf{x} - \mathbf{x}'|} = \frac{1}{r} + \frac{\mathbf{x}' \cdot \mathbf{x}}{r^3} + \frac{1}{2r^5} \sum_{ij} x_i x_j (3x_i' x_j' - r'^2 \delta_{ij}) + \cdots \qquad (4)$  $\Rightarrow \frac{1}{|\mathbf{x} - \mathbf{x}'|} = \frac{1}{|\mathbf{x} - \mathbf{x}_0|} - (\mathbf{x}' - \mathbf{x}_0) - (\mathbf{x}' - \mathbf{x}_0)$ On the RHS of (4), $\det \left\{ \mathbf{x} \to \mathbf{x} - \mathbf{x}_0 \\ \mathbf{x}' \to \mathbf{x}' - \mathbf{x}_0 \right\}$  $= \frac{1}{|\mathbf{x} - \mathbf{x}_0|} + \frac{(\mathbf{x}' - \mathbf{x}_0) \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} - (\mathbf{x}' - \mathbf{x}_0) \cdot (\mathbf{x}' - \mathbf{x}_0) - (\mathbf{x}' - \mathbf{x}_0)^2 \delta_{ij} + \cdots \qquad (4a)$  $+ \frac{1}{2} \sum_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} \left[ 3(x_i' - x_{0i})(x_j' - x_{0j}) - |\mathbf{x}' - \mathbf{x}_0|^2 \delta_{ij} + \cdots \qquad (4a)$ 

$$\Rightarrow \phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3x'$$

$$\stackrel{(4a)}{=} \frac{1}{4\pi\varepsilon_0} \left[ \frac{\int \rho(\mathbf{x}') d^3x'}{|\mathbf{x} - \mathbf{x}_0|} + \frac{(\mathbf{x} - \mathbf{x}_0) \cdot \int (\mathbf{x}' - \mathbf{x}_0) \rho(\mathbf{x}') d^3x'}{|\mathbf{x} - \mathbf{x}_0|^3} \underbrace{Q_{ij} \text{ w.r.t. } \mathbf{x}_0}_{\mathbf{y} - \mathbf{x}_0} \right] \frac{1}{2\pi\varepsilon_0} \left[ \frac{\mathbf{x} - \mathbf{x}_0 \cdot \mathbf{x}_0}{|\mathbf{x} - \mathbf{x}_0|^3} \int \left\{ 3(x_i' - x_{0i})(x_j' - x_{0j}) - |\mathbf{x}' - \mathbf{x}_0|^2 \delta_{ij} \right\} \rho(\mathbf{x}') d^3x' + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_0)(x_i - x_0)}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$

$$= \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x$$

In (5),  $\mathbf{p}$ ,  $Q_{ij}$ ,  $\cdots$  are defined w.r.t.  $\mathbf{x}_0$  and we may regard q,  $\mathbf{p}$ ,  $Q_{ij}$ , etc. to be located at  $\mathbf{x}_0$  [see p. 147, statement above (4.13)].

 $\mathbf{x}_0$  at or near the center of  $\rho$  can minimize higher moments. Why? At a large enough  $\mathbf{x}$ ,  $\phi(\mathbf{x})$  of the lowest moment dominates. Why?

*Exercise*: Prove that the lowest non-vanishing multipole moment is independent of the reference point (see pp. 147-8).

Solution: Each component of the  $\ell$ -th multipole moment w.r.t. reference points **a** & **b** consists, respectively, of integrals of the form

$$I_{ijk}^{(\mathbf{a})} = \int \rho(\mathbf{x})(x - a_x)^i (y - a_y)^j (z - a_z)^k d^3x \text{ and}$$

$$I_{ijk}^{(\mathbf{b})} = \int \rho(\mathbf{x})(x - b_x)^i (y - b_y)^j (z - b_z)^k d^3x$$

$$= \int \rho(\mathbf{x})(x - a_x - c_x)^i (y - a_y - c_y)^j (z - a_z - c_z)^k d^3x,$$

where i, j, and k are zero or positive integers  $(i + j + k = \ell)$ ,  $\mathbf{a} = (a_x, a_y, a_z)$ ,  $\mathbf{b} = (b_x, b_y, b_z)$ , and  $\mathbf{b} = \mathbf{a} + \mathbf{c}$  with  $\mathbf{c}$  given by  $\mathbf{c} = (c_x, c_y, c_z)$ .

having i + j + k = 2).

For example, the monopole moment has only one term (i = j = k = 0), each component x of the dipole moment consists of one term (i or j or k = 1), and each component of the quadrupole moment consists of multiple terms (all

### 4.1 Multipole Expansion (continued)

The monopole moment  $q = \int \rho(\mathbf{x}) d^3x$  is clearly indep. of the reference point. If q = 0 and if the lowest nonvanishing multipole moment w.r.t. reference point  $\mathbf{a}$  is the  $\ell$ -th moment, i.e.

$$I_{ijk}^{(\mathbf{a})} = \begin{cases} = 0, & i+j+k < l \\ \neq 0, & i+j+k = l \end{cases}$$
then, w.r.t. reference point **b**, we have
$$I_{ijk}^{(\mathbf{b})} = \int \rho(\mathbf{x}) \underbrace{(x - a_x - c_x)^i}_{=(x - a_x)^{i-}} \underbrace{(y - a_y - c_y)^j}_{=(y - a_y)^{j-}} \underbrace{(z - a_z - c_z)^k}_{=(z - a_z)^{k-}} d^3x$$

$$= \underbrace{(x - a_x)^{i-}}_{ic_x(x - a_x)^{i-1} + \dots} \underbrace{(y - a_y)^{j-1}}_{jc_y(y - a_y)^{j-1} + \dots} kc_z(z - a_z)^{k-1} + \dots$$

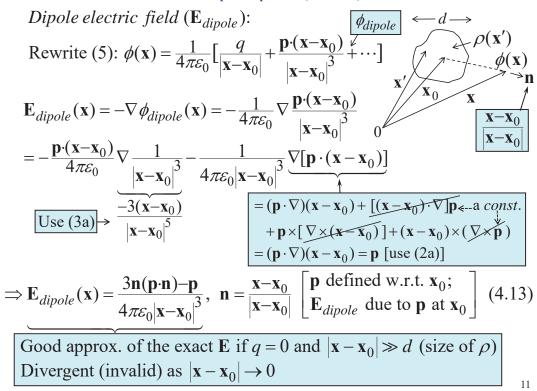
$$= \int_{i+j+k=l} \rho(\mathbf{x})(x - a_x)^i (y - a_y)^j (z - a_z)^k d^3x$$

$$+ \sum_{\alpha\beta\gamma} \underbrace{C_{\alpha\beta\gamma}}_{\alpha\beta\gamma} \int \rho(\mathbf{x})(x - a_x)^\alpha (y - a_y)^\beta (z - a_z)^\gamma d^3x$$

$$= I_{ijk}^{(\mathbf{a})} = 0$$

$$= I_{ijk}^{(\mathbf{a})} \underbrace{\int_{i+j+k=l}} e^{\mathbf{a}} \underbrace{\int_{i+j+k=l}} e^{\mathbf{$$

10



#### 4.1 Multipole Expansion (continued)

Discussion on reference point choice and field evaluation:

1. In 
$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \left( \frac{q}{r} + \frac{\mathbf{p} \cdot \mathbf{x}}{r^3} + \frac{1}{2r^5} \sum_{ij} Q_{ij} x_i x_j + \cdots \right) [(4.10)], \mathbf{p}, Q_{ij}, \text{ etc.}$$

are defined w.r.t.  $\mathbf{x} = 0$  and are put at  $\mathbf{x} = 0$  to evaluate  $\phi$ . In

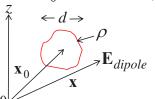
$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \left[ \frac{q}{|\mathbf{x} - \mathbf{x}_0|} + \frac{\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}_0)}{|\mathbf{x} - \mathbf{x}_0|^3} + \frac{1}{2} \sum_{ij} Q_{ij} \frac{(x_i - x_{0i})(x_j - x_{0j})}{|\mathbf{x} - \mathbf{x}_0|^5} + \cdots \right]$$
 [(5)],

**p**,  $Q_{ij}$ , etc. are defined w.r.t.  $\mathbf{x} = \mathbf{x}_0$  and are put at  $\mathbf{x} = \mathbf{x}_0$  to evaluate  $\phi$ .

p,  $Q_{ij}$ , etc. are defined ....

2. Define  $\mathbf{p}$ ,  $Q_{ij}$ , etc. w.r.t. a reference pt.

( $\mathbf{x}_0$ , right figure) located at or near the center ....  $\mathbf{E}_{dipole}$ 



3. The lowest non-vanishing moment gives the dominant contribution in the far zone. Although it is indep. of the reference pt., it is still desirable to put it at or near the center of  $\rho$  to evaluate  $\phi$ . For example, if q = 0, (4.10) and (5) give the same **p**, but

$$\mathbf{E}_{dipole}(\mathbf{x}) = \frac{3\mathbf{n}(\mathbf{p} \cdot \mathbf{n}) - \mathbf{p}}{4\pi\varepsilon_0 |\mathbf{x}|^3} \begin{bmatrix} \text{from} \\ (4.10) \end{bmatrix}; \ \mathbf{E}_{dipole}(\mathbf{x}) = \frac{3\mathbf{n}(\mathbf{p} \cdot \mathbf{n}) - \mathbf{p}}{4\pi\varepsilon_0 |\mathbf{x} - \mathbf{x}_0|^3} \begin{bmatrix} \text{from} \\ (5) \end{bmatrix}$$

#### 4.1 Multipole Expansion (continued)

(continued) Consider the same  $\rho$  as in last page. Since q = 0, **p** is indep. of the reference pt. (let it be  $\mathbf{p} = p\mathbf{e}_z$ ).

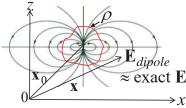
Case A: Put 
$$\mathbf{p} (= p\mathbf{e}_z)$$
 at  $\mathbf{x} = \mathbf{x}_0$ 

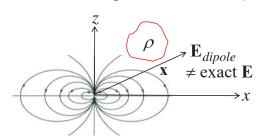
$$\Rightarrow \mathbf{E}_{dipole}(\mathbf{x}) = \frac{3\mathbf{n}(\mathbf{p} \cdot \mathbf{n}) - \mathbf{p}}{4\pi\varepsilon_0 |\mathbf{x} - \mathbf{x}_0|^3}$$
Case B: Put  $\mathbf{p} (= p\mathbf{e}_z)$  at  $\mathbf{x} = 0$ 

$$\Rightarrow \mathbf{E}_{dipole}(\mathbf{x}) = \frac{3\mathbf{n}(\mathbf{p} \cdot \mathbf{n}) - \mathbf{p}}{4\pi\varepsilon_0 |\mathbf{x}|^3}$$

Case A:  $\mathbf{E}_{dipole} \rightarrow \text{exact } \mathbf{E} \text{ at a}$ shorter distance from  $\rho$ 

Case B:  $\mathbf{E}_{dipole} \rightarrow \text{exact } \mathbf{E} \text{ at a}$ much larger distance from  $\rho$ 





# **4.2** Multipole Expansion of the Energy of a Charge Distribution in an External Field

In (1.53), we have  $W = \frac{1}{2} \int \rho(\mathbf{x}) \phi(\mathbf{x}) d^3 x \quad [\phi(\mathbf{x}) \text{ due to } \rho(\mathbf{x})]$   $\phi(\mathbf{x}) \text{ due to } \rho(\mathbf{x}) \text{ in the integrand; } \nabla^2 \phi(\mathbf{x}) = -\rho(\mathbf{x})/\varepsilon_0$ 

Here, we consider the energy of  $\rho(\mathbf{x})$  in  $\phi(\mathbf{x})$ , where  $\phi(\mathbf{x})$  is due to external charges:  $W = \int \rho(\mathbf{x})\phi(\mathbf{x})d^3x$  (4.21)

$$\phi(\mathbf{x})$$
 due to external charges;  $\nabla^2 \phi(\mathbf{x}) = 0$  in region of  $\rho(\mathbf{x})$ 

Expand the external field  $\phi(\mathbf{x})$  [Use (A.3) in appendix A]:

$$\phi(\mathbf{x}) = \phi(0) + \mathbf{x} \cdot \nabla \phi \Big|_{\mathbf{x}=0} + \frac{1}{2} \sum_{ij} x_i x_j \frac{\partial^2 \phi}{\partial x_i \partial x_j} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{2} \sum_{ij} x_i x_j \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

$$= \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left( 3x_i x_j - r^2 \delta_{ij} \right) \frac{\partial E_j}{\partial x_i} \Big|_{\mathbf{x}=0} + \cdots$$

13

Rewrite 
$$\phi(\mathbf{x}) = \phi(0) - \mathbf{x} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} \left(3x_i x_j - r^2 \delta_{ij}\right) \frac{\partial E_j(0)}{\partial x_i} + \cdots$$
 (4.23)

$$\Rightarrow W = \int \rho(\mathbf{x}) \phi(\mathbf{x}) d^3 x$$

$$= q \phi(0) - \mathbf{p} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} Q_{ij} \frac{\partial E_j(0)}{\partial x_i} + \cdots$$

$$\mathbf{p} = \int \mathbf{x} \rho(\mathbf{x}) d^3 x$$

$$(\mathbf{w.r.t.} \ \mathbf{x} = 0)$$

$$Q_{ij} = \int (3x_i x_j - r^2 \delta_{ij}) \rho(\mathbf{x}) d^3 x \quad (\mathbf{w.r.t.} \ \mathbf{x} = 0)$$

$$\phi(\mathbf{x}) \text{ due to charges external to } \rho.$$

$$\Rightarrow \begin{cases} q & [+] \text{ interacts with } \phi & \phi(\mathbf{x}) \text{ due to charges external to } \rho. \end{cases}$$

$$Q_{ij} = \int (3x_i x_j - r^2 \delta_{ij}) \rho(\mathbf{x}) d^3 x \quad (\mathbf{w.r.t.} \ \mathbf{x} = 0)$$

$$\Rightarrow \begin{cases} q & [+] \text{ interacts with } \mathbf{E} \text{ (non-uniform } \phi) \end{cases}$$

$$Q_{ij} = \int (3x_i x_j - r^2 \delta_{ij}) \rho(\mathbf{x}) d^3 x \quad (\mathbf{w.r.t.} \ \mathbf{x} = 0)$$

$$\Rightarrow \begin{cases} q & [+] \text{ interacts with } \mathbf{E} \text{ (non-uniform } \phi) \end{cases}$$

$$Q_{ij} = \int (3x_i x_j - r^2 \delta_{ij}) \rho(\mathbf{x}) d^3 x \quad (\mathbf{w.r.t.} \ \mathbf{x} = 0)$$

$$\Rightarrow \begin{cases} q & [+] \text{ interacts with } \mathbf{E} \text{ (non-uniform } \phi) \end{cases}$$

$$Q_{ij} = \int (3x_i x_j - r^2 \delta_{ij}) \rho(\mathbf{x}) d^3 x \quad (\mathbf{w.r.t.} \ \mathbf{x} = 0)$$

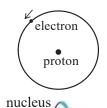
- 1. Higher order moments can "see" finer structure of  $\phi(\mathbf{x})$ . Why?
- 2. How does a charged rod attract a piece of paper?
- 3. How does a microwave oven heat food?

# 4.6 Models for the Molecular Polarizability

## **Induced Dipole Moment:**

Molecular (atomic) electrons obey the laws of quantum mechanics.

In the simplest case of a hydrogen atom, an electron (described by a wavefunction) rapidly moves around a proton. We ignore its orbital motion and consider only the motion of the orbital center, which coincides with the proton when there is no external **E**.



15

For most molecules/atoms (with few exceptions, e.g. water), there is 0 dipole moment in the absence of **E**(external). For simplicity, we may regard charges inside as e<sup>-</sup>/proton pairs. In the absence of **E**(external),

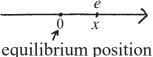


each pair are at the same equilibrium position, like a hydrogen atom.

Electrons and ions in a molecule (atom) are <u>bound charges</u>. In the presence of an external **E**, they (predominantly electrons) tend to be very slightly displaced from their equilibrium positions. The molecule (atom) is thus *polarized* (i.e. +) and dipole moments are *induced*.

#### 4.6 Models for the Molecular Polarizability (continued)

When a charge e is displaced from its equilibrium position (x = 0), it will be subject to a restoring force F(x), much like an object tied to a spring. We expand F(x) as



 $F(x) = F(0) + F'(0) \quad x + \frac{1}{2}F''(0)x^2 + \cdots$   $= 0 \quad = -m\omega_0^2 \quad \text{nonlinear effects, negligible if } x \to 0$ because x = 0 is the equilibrium position  $\omega_0$  is the natural frequency of e if it

oscillates as a simple harmonic oscillator.

Consider a charge e displaced from position 0 to x by force eE (e carries a sign). Assume F (restoring force) and x are along the same line (true for *isotropic* media), but in opposite directions.

For small 
$$\mathbf{x}$$
, we have  $\mathbf{F}(\mathbf{x}) \approx -m\omega_0^2 \mathbf{x}$  (4.71)  
Static balance  $\Rightarrow e\mathbf{E} + (-m\omega_0^2 \mathbf{x}) = 0 \Rightarrow \mathbf{x} = \frac{e}{m\omega_0^2} \mathbf{E}$ 
electric force restoring force

#### 4.6 Models for the Molecular Polarizability (continued)

Rewrite 
$$\mathbf{x} = \frac{e}{m\omega_0^2} \mathbf{E}$$

 $-m\omega_0^2 \mathbf{x} \stackrel{e}{\mathbf{x}} e \mathbf{E}$ 

This results in a dipole moment **p**:

 $\mathbf{p} = \int \mathbf{x}' \rho(\mathbf{x}') d^3 x' = \int \mathbf{x}' e \delta(\mathbf{x}' - \mathbf{x}) d^3 x = e \mathbf{x} = \frac{e^2}{m \omega_0^2} \mathbf{E} = \varepsilon_0 \gamma \mathbf{E}, \quad (4.72)$ 

where  $\gamma \equiv e^2/(\varepsilon_0 m \omega_0^2)$  is the polarizability for a *single* charge.

*Note*: **p** of a single charge (let it be an electron) depends on the reference point (it is x = 0 here). However, as discussed before, we match each electron with a proton (initially also at x = 0). Since the monopole is 0, the dipole moment is indep. of the reference pt.

 $\mathbf{p}_{mol}$  (molecular dipole moment) is the sum of all  $\mathbf{p}$  in a molecule:

$$\mathbf{p}_{mol} = \sum_{j} e_{j} \mathbf{x}_{j} = \sum_{j} \frac{e_{j}^{2}}{m_{j} \omega_{j}^{2}} \mathbf{E} = \varepsilon_{0} \gamma_{mol} \mathbf{E} \begin{bmatrix} \text{mostly due} \\ \text{to electrons} \end{bmatrix}$$
(4.72)+(4.73)

where 
$$\gamma_{mol} = \frac{1}{\varepsilon_0} \sum_{j} \frac{e_j^2}{m_j \omega_j^2} \left[ \underline{\text{molecular polarizability}} \right].$$
 (4.73)

*Note*: An *induced*  $\mathbf{p}_{mol}$  is  $\parallel$  to  $\mathbf{E}$ .  $\Rightarrow$  no touque on  $\mathbf{p}_{mol}$  (by  $\mathbf{E}$ )

Discussion:

(1)  $\mathbf{p} = e\mathbf{x}$  as calculated above for a single charge is with respect to the equilibrium position at x = 0. Different charges have different equilibrium positions. Thus, in  $\mathbf{p}_{mol} = \sum e_j \mathbf{x}_j$ , each  $e_j \mathbf{x}_j$  is with respect to a different reference point.

This will not cause any difficulty if the total + & – charges in the molecule are equal. Since the net charge is 0,  $\mathbf{p}_{mol}$  is the lowest non-vanishing moment, hence indep. of the reference point.

"Independent of the reference point" is a key to subsequent calculations. Thus, we assume that  $\mathbf{p}_{mol}$  is contributed by an equal amount of +/- charges in the molecule. If there is a net molecular charge, it will be treated separately [see (4.29) below].

(ii) The approximation made in (4.71),  $\mathbf{F}(\mathbf{x}) \approx -m\omega_0^2 \mathbf{x}$ , has led to a linear relation between  $\mathbf{p}_{mol}$  and  $\mathbf{E}$ , i.e.  $\mathbf{p}_{mol} = \varepsilon_0 \gamma_{mol} \mathbf{E}$ .

19

#### 4.6 Models for the Molecular Polarizability (continued)

*Problem*: A hydrogen atom is in an external  $E = 10^6$ V/m. Use  $p = \varepsilon_0 \gamma E$  [(4.72)] to get a crude estimate of the dipole moment p of this atom and the the electron displacement from its equilibrium position.



$$\begin{cases} \varepsilon_0 \approx 8.854 \times 10^{-12} \text{ F/m (p. 782)} \\ \gamma \approx 10^{-29} \text{ m}^3 \text{ (p. 163)} \end{cases} \Rightarrow \begin{cases} p \approx 8.854 \times 10^{-12} \times 10^{-29} \times 10^6 \\ \approx 8.9 \times 10^{-35} \text{ C-m} \end{cases}$$

Let d = the electron displacement from its equilibrium position.  $p = ed = 1.6 \times 10^{-19} d$  C-m (for  $E = 10^6$  V/m) extremely small!

$$\Rightarrow d = p / (1.6 \times 10^{-19}) \approx 8.9 \times 10^{-35} / (1.6 \times 10^{-19}) \approx 5.6 \times 10^{-16} \text{ m}$$

The water molecule has a permanent dipole moment of

$$p_{water} \approx 6.2 \times 10^{-30} \text{ C-m} [7 \times 10^4 \text{ times the } p \text{ in } E = 10^6 \text{ V/m}]$$

 $\Rightarrow$  To induce a p equal to  $p_{water}$  on the hydrogen atom, it requires an external  $E > 10^{10}$  V/m, which is  $\gg$  typical interatomic fields  $(10^5 - 10^8)$ V/m). So, well before E reaches this value, the hydrogen atom would be ionized (p would become a nonlinear function of E even sooner).  $_{20}$ 

## Permanent Dipole Moment under an E-Field:

Some molecules (like water) have a permanent dipole moment (**p**). These molecules are randomly oriented in the absence of an applied **E** so the *vector* sum of all permanent **p** over a small volume is 0, i.e.

$$\sum_{j} \mathbf{p}_{j} = 0 \quad [\mathbf{p}_{j}: \text{ same magnitude; random directions}]$$

$$\Rightarrow \langle \mathbf{p} \rangle = \frac{\sum_{j} \mathbf{p}_{j}}{\text{total no. of molecules}} = 0 \quad [\text{applied } \mathbf{E} = 0]$$



If the applied  $\mathbf{E} \neq 0$ , there will be a torque  $(\Gamma_E)$  on  $\mathbf{p}$ , which tends to align  $\mathbf{p}$  along  $\mathbf{E}$  (lower fig.). But a restoring torque  $(\Gamma_r)$  will restrict the rotation angle  $\theta$  to  $\theta \ll 1$  and the new equilibrium angle is  $\varphi + \theta$ , where  $\varphi$  is the original equilibrium angle. With  $\theta \ll 1$ , we have  $\Gamma_r \propto \theta$  (Taylor expansion) and  $\Gamma_E \propto E$ . Thus,  $\Gamma_r = \Gamma_E$  original equilibrium orientation (at  $\mathbf{E} = 0$ ) Unless  $\varphi = 90^\circ$ , a rotation tilts each  $\mathbf{p}$  toward  $\mathbf{E}$ . With  $\theta \ll 1$ , it's easy to show  $\mathbf{p}$  thus gains a  $\|$  component which is  $\propto \theta = \alpha E$  (How?). So  $\langle \mathbf{p} \rangle = (+const) \cdot \mathbf{E}$  [a linear relation as (4.72)]

#### **4.6 Models for the Molecular Polarizability** (continued)

## **Electric Polarization , Polarization Charge, and Free Charge:**

By (4.13), **E** of a *microscopic* molecular dipole  $(\mathbf{p}_{mol})$  z located at  $\mathbf{x} = 0$  is  $\mathbf{E}_{dipole} = \frac{3\mathbf{n}(\mathbf{p}_{mol} \cdot \mathbf{n}) - \mathbf{p}_{mol}}{4\pi\varepsilon_0 |\mathbf{x}|^3} [\mathbf{n} = \frac{\mathbf{x}}{|\mathbf{x}|}]$   $\mathbf{p}_{dipole} = p_{dipole}$ 

Good approx. of the exact **E** if  $|\mathbf{x}| \gg$  dipole size; divergent as  $|\mathbf{x}| \to 0$ 

We now define **P** (<u>electric polarization</u>, a *mascroscopic* quantity) as the total dipole mement per unit volume (due to bound charges):

sum over all types of molecules  $\mathbf{p}(\mathbf{x}) = \sum_{i}^{i} N_i(\mathbf{x}) \langle \mathbf{p}_i \rangle \leftarrow \mathbf{p}_i \text{ a small volume at } \mathbf{x}. \langle \mathbf{p}_i \rangle \text{ can be } \ll \mathbf{p}_i \text{ due to vector cancellation of, e.g. permanent } \mathbf{p}_i.$ 

 $P(\mathbf{x})$  gives no divergent  $\mathbf{E}$  at any  $\mathbf{x}$ , just like a macroscopic  $\rho(\mathbf{x})$  defined by  $\rho(\mathbf{x}) = N(\mathbf{x})q$  [ $N(\mathbf{x})$ : number density of point charges q] gives no divergent  $\mathbf{E}$  at any  $\mathbf{x}$  [see Exercise 2, Sec. 1.3].

Rewrite 
$$\mathbf{P}(\mathbf{x}) = \sum_{i} N_i(\mathbf{x}) \langle \mathbf{p}_i \rangle$$
 (4.28)

We now divide the charge density in a dielectric medium into two

categories: 
$$\begin{cases} \rho_{pol} \text{ (polarization charge density)} \\ \rho_{free} \text{ (free charge density)} \end{cases}$$

where  $ho_{pol}$  results from the separation of (equal)+/- bound charges in molecules, while  $\rho_{free}$  (if any) consists of (1) net molecular charges and (2) excess charges (such as free electrons) in the medium, i.e.

$$\rho_{free}(\mathbf{x}) = \sum_{i} N_{i}(\mathbf{x}) \langle e_{i} \rangle + \rho_{excess}(\mathbf{x}) \begin{bmatrix} \langle e_{i} \rangle : \text{ average net charge } \\ \text{ per type-} i \text{ molecule} \end{bmatrix}$$
(4.29)

*Example*: Some air molecules may contain a net charge  $e_i \ [ \Rightarrow \langle e_i \rangle ]$ . There are also a small number of free electrons in air [  $\Rightarrow \rho_{excess}(\mathbf{x})$ ].

*Note*:1.  $\langle e_i \rangle$  can be  $\ll e_i$  (e.g. 1 in  $10^6$  molecules contains a net  $e_i$ .)

2. We have used the notation  $\rho_{free}$  to distinguish it from  $\rho_{pol}$ .  $\rho_{free}$  here is denoted by  $\rho$  in Jackson [in (4.29), (4.35), etc.]

23

## 4.3 Elementary Treatment of Electrostatics with Ponderable Media

Macroscopic Version of  $\nabla \cdot \mathbf{E} = \rho / \varepsilon_0$  (for Dielectric Media):

Consider a medium with **P** (due to  $\rho_{pol}$ ) and  $\rho_{free}$ . We treat **P** (hence  $\rho_{pol}$ ) and  $\rho_{free}$  separately by expressing the potential  $[\Delta \phi(\mathbf{x})]$ due to charges in a small volume  $\Delta V$  at  $\mathbf{x}'$  as

$$\Delta \phi(\mathbf{x}) = \Delta \phi_{free}(\mathbf{x}) + \Delta \phi_{pol}(\mathbf{x}),$$

$$\Delta \phi(\mathbf{x}) = \Delta \phi_{free}(\mathbf{x}) + \Delta \phi_{pol}(\mathbf{x}),$$
where  $\Delta \phi_{free}$  is due to  $\rho_{free}(\mathbf{x}')\Delta V$  and  $\Delta \phi_{pol}$  is due
to  $\rho_{pol}(\mathbf{x}')\Delta V$ . Clearly,  $\Delta \phi_{free}(\mathbf{x}) = \frac{1}{4\pi\mathcal{E}_0} \frac{\rho_{free}(\mathbf{x}')\Delta V}{|\mathbf{x} - \mathbf{x}'|}$ .

For  $\Delta \phi$ , we don't yet have an expression for  $\rho$ .

For  $\Delta \phi_{pol}$ , we don't yet have an expression for  $\rho_{pol}$ .

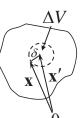
So we use (5): 
$$\frac{q_{pol} = \int \rho_{pol}(\mathbf{x}) d^3 x = 0}{4\pi\varepsilon_0} \left[ \frac{q_{pol}}{|\mathbf{x} - \mathbf{x}'|} + \frac{\mathbf{P}(\mathbf{x}')\Delta V \cdot (\mathbf{x} - \mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|^3} + \cdots \right] \approx \frac{\mathbf{P}(\mathbf{x}')\Delta V \cdot (\mathbf{x} - \mathbf{x}')}{4\pi\varepsilon_0 |\mathbf{x} - \mathbf{x}'|^3} \quad (6)$$

#### 4.3 Elementary Treatment of Electrostatics with Ponderable Media (continued)

Rewrite 
$$\Delta \phi_{pol}(\mathbf{x}) \approx \frac{g_{pol}}{4\pi\varepsilon_0 |\mathbf{x} - \mathbf{x}'|} + \frac{\mathbf{P}(\mathbf{x}')\Delta V \cdot (\mathbf{x} - \mathbf{x}')}{4\pi\varepsilon_0 |\mathbf{x} - \mathbf{x}'|^3} + \begin{pmatrix} \text{higher order} \\ \text{terms} \end{pmatrix} [(6)]$$

*Question* 1: Will  $\Delta \phi_{pol}(\mathbf{x})$  be divergent as  $\mathbf{x} \to \mathbf{x}'$ ?

Ans.: Let  $|\mathbf{x} - \mathbf{x}'| = \delta$  with  $\delta \to 0$ . Let  $\Delta V$  be a sphere of radius  $\delta$  centered at  $\mathbf{x}'$ . So  $\mathbf{x}$  is a point on the spherical surface. Then, in (6),  $\Delta V \propto \delta^3$  and  $\frac{\mathbf{x} - \mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|^3} \propto \frac{1}{\delta^2}$ 



- $\Rightarrow \Delta \phi_{pol}(\mathbf{x})$  (due to nearby dipoles in the sphere)  $\propto \delta \rightarrow 0$
- $\Rightarrow$  The macroscopic **P** makes the dipole term non-divergent.
- $\Rightarrow$   $\phi_{pol}(\mathbf{x})$  are contributed mostly by dipoles farther away from  $\mathbf{x}$ .

Question 2: What's the meaning of neglecting higher-order terms?

Ans.: Higher-order terms contribute mostly to the extremely large microscopic fields inside molecules, which are of no interest to us. Fields outside the charge-neutral molecules are much smaller. Outside the molecules, the dipole term is dominant. Higher-order terms fall off much faster with distance than the dipole term, so we just neglect them.

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#### 4.3 Elementary Treatment of Electrostatics with Ponderable Media (continued)

$$\Delta\phi_{free}(\mathbf{x}) = \frac{1}{4\pi\varepsilon_{0}} \frac{\rho_{free}(\mathbf{x}')\Delta V}{|\mathbf{x}-\mathbf{x}'|} \text{ and } \Delta\phi_{pol}(\mathbf{x}) = \frac{\mathbf{P}(\mathbf{x}')\Delta V \cdot (\mathbf{x}-\mathbf{x}')}{4\pi\varepsilon_{0}|\mathbf{x}-\mathbf{x}'|^{3}}$$

$$\Rightarrow \Delta\phi(\mathbf{x}) = \Delta\phi_{free} + \Delta\phi_{pol} = \frac{1}{4\pi\varepsilon_{0}} \left[ \frac{\rho_{free}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \frac{\mathbf{P}(\mathbf{x}') \cdot (\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^{3}} \right] \Delta V \quad (4.30)$$
Let  $\Delta V \to d^{3}x'$ , use  $\frac{\mathbf{x}-\mathbf{x}'}{|\mathbf{x}-\mathbf{x}'|^{3}} = \nabla' \frac{1}{|\mathbf{x}-\mathbf{x}'|}$ , and integrate over volume
$$\Rightarrow \phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_{0}} \int \left[ \frac{\rho_{free}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} + \mathbf{P}(\mathbf{x}') \cdot \nabla' \frac{1}{|\mathbf{x}-\mathbf{x}'|} \right] d^{3}x', \quad \left[ = \oint_{S} \frac{\mathbf{P}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \cdot d\mathbf{a}' = 0 \right] \left[ \mathbf{P} = 0 \text{ on } S \text{ as } S \to \infty \right]$$
where  $\int \mathbf{P}(\mathbf{x}') \cdot \nabla' \frac{1}{|\mathbf{x}-\mathbf{x}'|} d^{3}x' \stackrel{!}{=} -\int \frac{\nabla' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} d^{3}x' + \int \nabla' \cdot \left( \frac{\mathbf{P}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} \right) d^{3}x' \right]$ 

$$= -\frac{1}{4\pi\varepsilon_{0}} \int \frac{\nabla' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|} d^{3}x' \stackrel{!}{=} -\int \frac{\Delta V}{|\mathbf{x}-\mathbf{x}'|} d^{3}x' \stackrel{!}{=} -\frac{\Delta V}{|\mathbf{x}-\mathbf{x}$$

#### 4.3 Elementary Treatment of Electrostatics with Ponderable Media (continued)

Rewrite: 
$$\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho_{free}(\mathbf{x}') - \nabla' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d^3x'$$
 (4.32)

$$\Rightarrow \underbrace{\nabla^{2} \phi(\mathbf{x})}_{-\nabla \cdot \mathbf{E}(\mathbf{x})} = \frac{1}{4\pi\varepsilon_{0}} \int [\rho_{free}(\mathbf{x}') - \nabla' \cdot \mathbf{P}(\mathbf{x}')] \underbrace{\nabla^{2} \frac{1}{|\mathbf{x} - \mathbf{x}'|}}_{-4\pi\delta(\mathbf{x} - \mathbf{x}')} d^{3}x'$$

$$\Rightarrow \nabla \cdot \mathbf{E}(\mathbf{x}) = \frac{1}{\varepsilon_{0}} [\rho_{free}(\mathbf{x}) - \nabla \cdot \mathbf{P}(\mathbf{x})]$$
(4.33)

In electrostatics, only electric charges can produce E. The equal footing of  $\rho_{free}$  and  $-\nabla \cdot \mathbf{P}$  in (4.32) and (4.33) suggests that  $-\nabla \cdot \mathbf{P}$ must represent a charge density (see p. 153 and p. 156). Thus, (4.33) can be written

$$\nabla \cdot \mathbf{E}(\mathbf{x}) = \frac{1}{\varepsilon_0} [\rho_{free}(\mathbf{x}) + \rho_{pol}(\mathbf{x})]$$
with  $\rho_{pol}(\mathbf{x}) = -\nabla \cdot \mathbf{P}(\mathbf{x})$  [polarization charge density]

A direct derivation of (7) can be

found in Appendix B [see Eq. (B.2)].

#### 4.3 Elementary Treatment of Electrostatics with Ponderable Media (continued)

Define an electric displacement (**D**) as  $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$ 

We may put  $\nabla \cdot \mathbf{E}(\mathbf{x}) = \frac{1}{\varepsilon_0} [\rho_{free}(\mathbf{x}) - \nabla \cdot \mathbf{P}(\mathbf{x})] [(4.33)]$  in the form:

$$\nabla \cdot \mathbf{D}(\mathbf{x}) = \rho_{free}(\mathbf{x})$$
 [applicable to dielectric media] (4.35)

**Dielectric Constant**: For an isotropic medium, the (approximate) linear relation  $\mathbf{F}(x) \approx -m\omega_0^2 \mathbf{x}$  [(4.71)] has led to the linear relation of  $\mathbf{p}_{mol} = \varepsilon_0 \gamma_{mol} \mathbf{E}$  [(4.72)+(4.73)] for a *single* molecule. So, **P** (the sum of all  $\mathbf{p}_{mol}$  per unit volume) and  $\mathbf{E}$  must also have a linear relation:

$$\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E},\tag{4.36}$$

where  $\chi_e$  in the proportionality constant is the electric susceptibility.

Sub. 
$$\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E}$$
 [(4.36)] into  $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P}$  [(4.34)], we obtain

$$\mathbf{D} = \varepsilon \mathbf{E},\tag{4.37}$$

$$\begin{cases} (4.34) \\ (4.37) \end{cases} \Rightarrow \mathbf{P} = (\varepsilon - \varepsilon_0) \mathbf{E}$$

where  $\varepsilon = \varepsilon_0 (1 + \chi_e)$   $\begin{cases} (4.34) \\ (4.37) \end{cases} \Rightarrow \mathbf{P} = (\varepsilon - \varepsilon_0) \mathbf{E}$   $\varepsilon : \underline{\text{electric permittivity}}$   $\varepsilon \in \varepsilon_0 : \underline{\text{dielectric constant or relative electric permittivity}}$ 

(4.38)

27

(8)

*Question*: Does **D** have a physical meaning?

#### 4.3 Elementary Treatment of Electrostatics with Ponderable Media (continued)

Discussion:  $\varepsilon$  is a macroscopic property of a medium derived from the microscopic behavior of molecular/atomic electrons. It is usually obtained by measurement and tabulated in handbooks.

Examples:  $\varepsilon(\text{air}) \approx 1.0006\varepsilon_0$ ,  $\varepsilon(\text{teflon}) \approx 2\varepsilon_0$ ,  $\varepsilon(\text{water}) \approx 80\varepsilon_0$ Special case: For a uniform medium,  $\varepsilon$  is independent of **x**.

$$\Rightarrow \qquad \nabla \cdot \mathbf{D} = \nabla \cdot \varepsilon \mathbf{E} = \varepsilon \nabla \cdot \mathbf{E} = \rho_{free}$$

$$\Rightarrow \qquad \nabla \cdot \mathbf{E} = \frac{\rho_{free}}{\varepsilon} \begin{bmatrix} \text{for } \rho_{free} & \text{in a uniform } \\ \text{dielectric medium} \end{bmatrix}$$
(4.39)

Compare (4.39) with (1.13):

$$\nabla \cdot \mathbf{E} = \frac{\rho_{free}}{\varepsilon_0} \begin{bmatrix} \text{for } \rho_{free} & \text{in } \\ \text{free space} \end{bmatrix} \qquad \mathbf{E} \text{ (due to } Q) \longrightarrow (1.13)$$

$$\Rightarrow \text{ In a uniform medium}$$

$$\text{with } \varepsilon > \varepsilon_0 \text{ (usual case)},$$

$$\rho_{free} \text{ produces } \frac{\varepsilon_0}{\varepsilon} \text{ of the}$$

$$\mathbf{E} \text{ it produces in free space.}$$

$$\varepsilon > \varepsilon_0 \text{ medium}$$

4.3 Elementary Treatment of Electrostatics with Ponderable Media (continued)

## Conversion of $\varepsilon$ to the Gaussian System:

 $\varepsilon$  in the SI system is called the electric permittivity ( $\varepsilon = \varepsilon_0$  for the free-space). It has no counterpart in the Gaussian system. However,  $\varepsilon/\varepsilon_0$  in the SI system (called dielectric constant or relative permittivity, see p.154) has a counterpart denoted by  $\varepsilon$  in the Gaussian system (a dimensionless quantity,  $\varepsilon = 1$  for the free-space).

P. 782 gives the conversion formula:

$$\begin{bmatrix} \text{Gaussian} \\ \varepsilon \end{bmatrix} \Leftrightarrow \begin{bmatrix} \text{SI} \\ \varepsilon/\varepsilon_0 \end{bmatrix}$$

Although  $\varepsilon$  in the Gaussian system has the same notation as the electric permittivity of the SI system, it is really the dielectric constant  $\varepsilon/\varepsilon_0$  of the SI system. Thus,  $\varepsilon$  in these two systems are related, but not the same physical quantity.

## 4.4 Boundary-Value Problems with Dielectrics

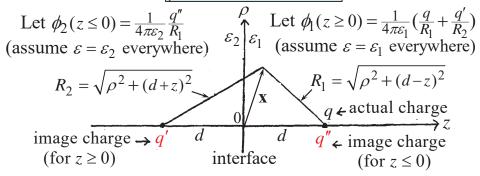
b.c.'s: [Derived as (1.22) in lecture notes.  $\sigma_{free}$  here is  $\sigma$  in (4.40)]

(i) 
$$\nabla \cdot \mathbf{D} = \rho_{free}$$
 [(4.35)]  $\rho_{\perp 2}$   $\rho_{free}$  (ii)  $\nabla \times \mathbf{E} = 0$   $\rho_{free}$   $\rho_{\perp 2}$   $\rho_{\perp 1}$   $\rho_{\perp 1}$   $\rho_{\perp 1}$   $\rho_{\perp 1}$   $\rho_{\perp 1}$   $\rho_{\perp 2}$   $\rho_{free}$   $\rho_{free}$   $\rho_{free}$   $\rho_{\perp 2}$   $\rho_{free}$ 

*Problem 1*: Two semi-infinite dielectrics have an interface plane at z = 0. A point charge q is at z = d. Find  $\phi$ ,  $\sigma_{pol}$ , and  $\rho_{pol}$  everywhere.

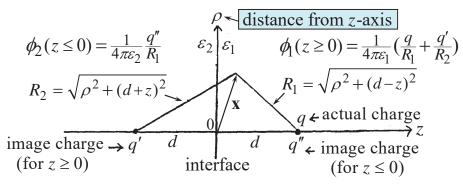
Calculating  $\phi$ : For  $\phi(z \ge 0)$ , put an image charge q' at z = -d on the z-axis. For  $\phi(z \le 0)$ , put an image charge q'' at z = d on the z-axis.

### $\rho$ : distance from z-axis



31

#### 4.4 Boundary-Value Problems with Dielectrics (continued)



Apply b.c.'s at z = 0.

b.c. 1: 
$$\varepsilon_{1}E_{\perp 1} - \varepsilon_{2}E_{\perp 2} = \sigma_{free} = 0 \implies \varepsilon_{1}\frac{\partial\phi_{1}}{\partial z}\Big|_{z=0} = \varepsilon_{2}\frac{\partial\phi_{2}}{\partial z}\Big|_{z=0}$$

$$\Rightarrow \left[q\frac{\partial}{\partial z}\frac{1}{R_{1}} + q'\frac{\partial}{\partial z}\frac{1}{R_{2}}\right]_{z=0} = q''\frac{\partial}{\partial z}\frac{1}{R_{1}}\Big|_{z=0} \implies q-q'=q''$$
b.c. 2:  $E_{t1} = E_{t2} \implies \frac{\partial\phi_{1}}{\partial\rho}\Big|_{z=0} = \frac{\partial\phi_{2}}{\partial\rho}\Big|_{z=0} = \frac{E_{\perp}}{E_{t}}: \text{ normal to interface}$ 

$$\Rightarrow \frac{1}{\varepsilon_{1}}\left[q\frac{\partial}{\partial\rho}\frac{1}{R_{1}} + q'\frac{\partial}{\partial\rho}\frac{1}{R_{2}}\right]_{z=0} = \frac{1}{\varepsilon_{2}}q''\frac{\partial}{\partial\rho}\frac{1}{R_{1}}\Big|_{z=0} \implies \frac{1}{\varepsilon_{1}}(q+q') = \frac{1}{\varepsilon_{2}}q''$$

$$\phi_{2}(z \leq 0) = \frac{q}{4\pi} \frac{2}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{1}} \quad \varepsilon_{2} \quad \varepsilon_{1} \quad \phi_{1}(z \geq 0) = \frac{q}{4\pi\varepsilon_{1}} \left(\frac{1}{R_{1}} - \frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{2}}\right)$$

$$R_{2} = \sqrt{\rho^{2} + (d + z)^{2}} \quad R_{1} = \sqrt{\rho^{2} + (d - z)^{2}} \quad q \in \text{actual charge}$$

$$\text{image charge} \rightarrow q' \quad d \quad q'' \in \text{image charge}$$

$$\text{(for } z \geq 0) \quad \text{interface} \quad \text{(for } z \leq 0)$$

$$\begin{cases} q - q' = q'' \\ \frac{1}{\varepsilon_{1}}(q + q') = \frac{1}{\varepsilon_{2}}q'' \end{cases} \Rightarrow q' = -\frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{2} + \varepsilon_{1}}q \quad \& \quad q'' = \frac{2\varepsilon_{2}}{\varepsilon_{2} + \varepsilon_{1}}q \quad (4.45)$$

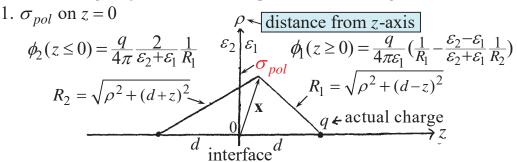
$$\Rightarrow \begin{cases} \phi_{1}(z \geq 0) = \frac{q}{4\pi\varepsilon_{1}} \left(\frac{1}{R_{1}} - \frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{2}}\right) \\ \phi_{2}(z \leq 0) = \frac{q}{4\pi} \frac{2}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{1}} \end{cases} \quad \text{(At } z = 0, \ R_{1} = R_{2}. \Rightarrow \phi_{1} = \phi_{2} \\ \therefore E \text{ is finite at the interface.} \end{cases}$$

 $\phi_1$ ,  $\phi_2$  obviously satisfy the Poisson Eq., hence are unique solutions.

33

#### 4.4 Boundary-Value Problems with Dielectrics (continued)

Calculating surface and volume polarization charges:



From (8): 
$$\begin{cases} \mathbf{P}_1 = (\varepsilon_1 - \varepsilon_0)\mathbf{E}_1 = -(\varepsilon_1 - \varepsilon_0)\nabla\phi_1 \\ \mathbf{P}_2 = (\varepsilon_2 - \varepsilon_0)\mathbf{E}_2 = -(\varepsilon_2 - \varepsilon_0)\nabla\phi_2 \end{cases} \begin{bmatrix} \mathbf{P}_1, \mathbf{P}_2 \text{ are given by } \phi_1, \phi_2 \text{ above.} \end{bmatrix}$$

To find  $\sigma_{pol}$  on the interface, draw a thin pillbox of small area A on the interface and apply the divergence thm.:  $\sigma_{pol} A$   $\int_{\mathcal{V}} \nabla \cdot \mathbf{P} d^3 x = \oint_{\mathcal{S}} \mathbf{P} \cdot \mathbf{n} da \implies -Q_{pol} = [\mathbf{P}_2 - \mathbf{P}_1]_{z=0} \cdot \mathbf{n} A \qquad \mathbf{n} \leftarrow \mathbf{P} A \rightarrow \mathbf{n} A$   $\Rightarrow \sigma_{pol} = \frac{Q_{pol}}{A} = -[\mathbf{P}_2 - \mathbf{P}_1]_{z=0} \cdot \mathbf{n} = -\frac{q}{2\pi} \frac{\varepsilon_0 (\varepsilon_2 - \varepsilon_1)}{\varepsilon_1 (\varepsilon_2 + \varepsilon_1)} \frac{d}{(\rho^2 + d^2)^{3/2}} \qquad (4.47)$ 

#### 4.4 Boundary-Value Problems with Dielectrics (continued)

2. 
$$\rho_{pol}$$
 in  $z > 0$ 

$$\phi_{2}(z \le 0) = \frac{q}{4\pi} \frac{2}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{1}}$$

$$\varepsilon_{2} = \frac{q}{4\pi \varepsilon_{1}} \frac{2}{R_{1}} \frac{1}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{1}}$$

$$\varepsilon_{2} = \frac{q}{4\pi \varepsilon_{1}} \frac{2}{R_{1}} \frac{1}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{2}}$$

$$R_{1} = \sqrt{\rho^{2} + (d - z)^{2}} \left[ = |\mathbf{x} - d\mathbf{e}_{z}| \right]$$

$$= |\mathbf{x} + d\mathbf{e}_{z}|$$

$$q^{\prime} = \frac{q}{4\pi \varepsilon_{1}} \left( \frac{1}{R_{1}} - \frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{R_{2}} \right) = \frac{q}{4\pi \varepsilon_{1}} \left( \frac{1}{|\mathbf{x} - d\mathbf{e}_{z}|} - \frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{|\mathbf{x} + d\mathbf{e}_{z}|} \right)$$

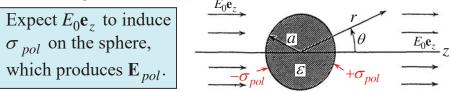
$$\Rightarrow \rho_{pol}(z > 0) = -\nabla \cdot \mathbf{P}_{1}^{(8)} = -(\varepsilon_{1} - \varepsilon_{0})\nabla \cdot \mathbf{E}_{1} = (\varepsilon_{1} - \varepsilon_{0})\nabla^{2}\phi_{1}$$

$$\nabla^{2} \frac{1}{|\mathbf{x} - \mathbf{x}'|} = -q \frac{\varepsilon_{1} - \varepsilon_{0}}{\varepsilon_{1}} [\delta(\mathbf{x} - d\mathbf{e}_{z}) - \frac{\varepsilon_{2} - \varepsilon_{1}}{\varepsilon_{2} + \varepsilon_{1}} \frac{\delta(\mathbf{x} + d\mathbf{e}_{z})}{\varepsilon_{2} + \varepsilon_{1}} \frac{1}{\varepsilon_{2} + \varepsilon_{$$

- $\Rightarrow$  There is a  $q_{pol} = -q(1 \frac{\mathcal{E}_0}{\mathcal{E}_1})$  at the same position  $(\mathbf{x} = d\mathbf{e}_z)$  as q.
- $\Rightarrow q_{pol} + q = q \frac{\varepsilon_0}{\varepsilon_1} \Rightarrow \text{If } \varepsilon_1 > \varepsilon_0$  (usual case),  $q_{pol}$  partially offsets q. Similarly, we can show  $\rho_{pol} = 0$  everywhere in the region z < 0.

#### 4.4 Boundary-Value Problems with Dielectrics (continued)

*Problem 2*: A uniform dielectric sphere is placed in a uniform electric field  $E_0\mathbf{e}_z$ . Find  $\phi$  and polarization charges everywhere



Divide the space into 2 regions: r < a and r > a. In both regions, we

have 
$$\nabla \cdot \mathbf{E} = \begin{cases} \rho_{free} / \varepsilon \ (r < a) \ [(4.39)] \\ \rho_{free} / \varepsilon_0 (r > a) \ [(1.13)] \end{cases}$$
.  $\rho_{free} = 0 \Rightarrow \nabla^2 \phi = 0 \begin{bmatrix} \text{for } r < a \\ \& r > a \end{bmatrix}$ 

$$\Rightarrow \phi = \begin{cases} r^{l} \\ r^{-l-1} \end{cases} \begin{cases} P_{\nu}^{m}(\cos \theta) \\ Q_{\nu}^{m}(\cos \theta) \end{cases} \begin{cases} e^{im\varphi} \\ e^{-im\varphi} \end{cases}$$
 [in spherical coordinates; see Sec. 3.1 of lecture notes]

b.c. 
$$\begin{cases} \phi \text{ is independent of } \phi. \\ \phi \text{ is finite at } \cos \theta = \pm 1. \end{cases} \Rightarrow \begin{cases} \phi_{in} = \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta) \\ \phi_{out} = \sum_{l=0}^{\infty} \left[ B_l r^l + C_l r^{-l-1} \right] P_l(\cos \theta) \end{cases}$$

#### **4.4 Boundary-Value Problems with Dielectrics** (continued)

Rewrite: 
$$\phi_{in} = \sum_{l=0}^{\infty} A_l r^l P_l(\cos \theta)$$
,  $\phi_{out} = \sum_{l=0}^{\infty} \left[ B_l r^l + C_l r^{-l-1} \right] P_l(\cos \theta)$   
b.c. (i):  $\phi_{out}(\infty) = -E_0 r \cos \theta \Rightarrow B_1 = -E_0$ ;  $B_l(l \neq 1) = 0$ 
b.c. (ii):  $\phi_{in}(a) = \phi_{out}(a)$  [  $\Rightarrow E_t^{in}(a) = E_t^{out}(a)$ ]

$$\Rightarrow A_{l}a^{l} = B_{l}a^{l} + \frac{C_{l}}{a^{l+1}} \Rightarrow \begin{cases} A_{1} = -E_{0} + \frac{C_{1}}{a^{3}} \\ A_{l} = \frac{C_{l}}{a^{2l+1}}, \ l \neq 1 \end{cases} \xrightarrow{a \in \mathcal{E}_{0}} \mathbf{e}_{z}$$
(9)

b.c. (iii): 
$$\varepsilon E_r^{in}(a) = \varepsilon_0 E_r^{out}(a) \Rightarrow -\varepsilon \frac{\partial}{\partial r} \phi_{in} \Big|_{r=a} = -\varepsilon_0 \frac{\partial}{\partial r} \phi_{out} \Big|_{r=a}$$

$$\Rightarrow \varepsilon l A_l a^{l-1} = \varepsilon_0 \left[ l B_l a^{l-1} - \frac{(l+1)C_l}{a^{l+2}} \right] \Rightarrow \begin{cases} \varepsilon A_l = -\varepsilon_0 \left[ E_0 + \frac{2C_1}{a^3} \right] & (11) \\ \varepsilon l A_l = -\varepsilon_0 \frac{(l+1)C_l}{a^{2l+1}}, \ l \neq 1 \end{cases}$$

$$(9), (11) \Rightarrow A_1 = -\frac{3}{\varepsilon/\varepsilon_0 + 2} E_0; \ C_1 = \left(\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2}\right) a^3 E_0$$

$$(10), (12) \Rightarrow A_l = C_l = 0 \text{ for } l \neq 1$$

37

#### 4.4 Boundary-Value Problems with Dielectrics (continued)

$$\Rightarrow \begin{cases} \phi_{in} = \phi(r \le a) = -\frac{3}{\frac{\mathcal{E}}{\mathcal{E}_{0}} + 2} E_{0} r \cos \theta \ [ = \phi \text{ of } E_{0} \mathbf{e}_{z} + \phi \text{ due to } \sigma_{pol} ] \\ \phi_{out} = \phi(r \ge a) = -E_{0} r \cos \theta + \frac{\frac{\mathcal{E}}{\mathcal{E}_{0}} - 1}{\frac{\mathcal{E}}{\mathcal{E}_{0}} + 2} E_{0} \frac{a^{3}}{r^{2}} \cos \theta \\ \phi \text{ of } E_{0} \mathbf{e}_{z} & \phi \text{ due to } \sigma_{pol} \end{cases} \xrightarrow{\boldsymbol{e}_{z}} \boldsymbol{e}_{z}$$

Comparing (4.54) with (4.10):  $\phi(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0} \left( \frac{q}{r} + \frac{\mathbf{p} \cdot \mathbf{x}}{r^3} + \frac{1}{2r^5} \ddot{\mathbf{Q}} \cdot \mathbf{x}\mathbf{x} + \cdots \right)$ 

we find  $\phi(r \ge a)$  due to  $\sigma_{pol}$  is exactly the  $\phi$  of the dipole term with

$$\mathbf{p} = 4\pi a^{3} \varepsilon_{0} \frac{\frac{\mathcal{E}}{\mathcal{E}_{0}} - 1}{\frac{\mathcal{E}}{\mathcal{E}_{0}} + 2} E_{0} \mathbf{e}_{z} \quad [\text{with } q, \ddot{\mathbf{Q}} \cdots, etc. = 0]$$
(4.56)

 $\Rightarrow$  The dipole field (for  $r \ge a$ ) is an exact expression even as  $r \to a$ .

For 
$$r \le a$$
,  $\phi_{in} \Rightarrow \mathbf{E}_{in} = \frac{3E_0}{\frac{\mathcal{E}}{\mathcal{E}_0} + 2} \mathbf{e}_z \Rightarrow \sigma_{pol}$  on the sphere produces a

uniform  $E_z$  inside the sphere. If  $\varepsilon > \varepsilon_0$  (usual case), we have  $\mathbf{E}_{in} < E_0 \mathbf{e}_z$ .

 $\Rightarrow$  E due to  $\sigma_{pol}$  cancels part of the external  $E_0 \mathbf{e}_z$ .

#### 4.4 Boundary-Value Problems with Dielectrics (continued)

$$\phi \text{ in (4.54)} \Rightarrow \begin{cases}
\mathbf{E}_{in} = \frac{3E_0}{\varepsilon/\varepsilon_0 + 2} \mathbf{e}_z \text{ (uniform)} \\
\mathbf{E}_{out} = E_0 \mathbf{e}_z + \frac{3\mathbf{e}_r(\mathbf{p} \cdot \mathbf{e}_r) - \mathbf{p}}{4\pi\varepsilon_0 r^3} \begin{bmatrix} \text{same form} \\ \text{as (4.13)} \end{bmatrix} \text{ with } \mathbf{e}_r = \frac{\mathbf{x}}{|\mathbf{x}|} \\
\Rightarrow \mathbf{P} = (\varepsilon - \varepsilon_0) \mathbf{E}_{in} = 3\varepsilon_0 (\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2}) E_0 \mathbf{e}_z \begin{bmatrix} \mathbf{P} \text{ (total } \mathbf{p} \text{ per unit volume)} \\ \text{volume)} \text{ is uniform.} \end{bmatrix} (4.57)$$

*Exercise*: Show that  $\mathbf{p}$  in (4.56) is indeed the total dipole moment.

$$\mathbf{p} = \frac{4\pi a^3}{3} \mathbf{P} \Rightarrow \mathbf{p} = 4\pi a^3 \varepsilon_0 \left( \frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2} \right) E_0 \mathbf{e}_z \text{ [same as (4.56)]}$$

Rewrite  $\nabla \cdot \mathbf{P} = -\rho_{nol} [(7)]$ 

**P** is uniform inside the sphere.  $\Rightarrow \rho_{pol}(r < a) = -\nabla \cdot \mathbf{P} = 0$ .

To find  $\sigma_{pol}$  due to the discontinuity of **P** at r = a,

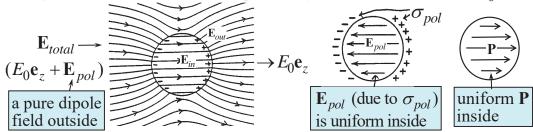
To find 
$$\sigma_{pol}$$
 due to the discontinuity of  $\mathbf{P}$  at  $r = a$ ,  $\mathbf{P}_{out} = 0$  draw a pillbox at  $r = a$  and apply the divergence thm.:
$$\int_{V} \nabla \cdot \mathbf{P} d^{3}x = \oint_{S} \mathbf{P} \cdot \mathbf{e}_{r} da.$$

$$\Rightarrow \sigma_{pol} = -(\mathbf{P}_{out} - \mathbf{P}) \cdot \mathbf{e}_{r} = P \cos \theta = 3\varepsilon_{0} (\frac{\varepsilon/\varepsilon_{0} - 1}{\varepsilon/\varepsilon_{0} + 2}) E_{0} \cos \theta \qquad (4.58)$$

$$\Rightarrow \sigma_{pol} = -(\mathbf{P}_{out} - \mathbf{P}) \cdot \mathbf{e}_r = P \cos \theta = 3\varepsilon_0 (\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2}) E_0 \cos \theta \qquad (4.58)$$

#### 4.4 Boundary-Value Problems with Dielectrics (continued)

Figures below show the field patterns just calculated (for  $\varepsilon > \varepsilon_0$ ).



field outside is uniform inside inside

Exercise: Show that 
$$\mathbf{p}$$
 in (4.56) agrees with  $\mathbf{p} = \int \mathbf{x} \rho(\mathbf{x}) d^3 x$ .

Let 
$$\begin{cases} \rho_{pol}(\mathbf{x}) = \sigma_{pol} \delta(r - a) = 3\varepsilon_0 (\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2}) E_0 \cos \theta \delta(r - a) & \theta \\ \mathbf{x} = r\mathbf{e}_r = r[\cos \theta \mathbf{e}_z + \sin \theta(\cos \varphi \mathbf{e}_x + \sin \varphi \mathbf{e}_y)] & \theta \end{cases}$$

$$\Rightarrow \mathbf{p} = \int \mathbf{x} \rho_{pol}(\mathbf{x}) d^3 x$$

$$= \int_0^\infty r^2 dr \int_{-1}^1 d(\cos \theta) \int_0^{2\pi} d\varphi \ r[\cos \theta \mathbf{e}_z + \sin \theta(\cos \varphi \mathbf{e}_x + \sin \varphi \mathbf{e}_y)] \\ \cdot 3\varepsilon_0 (\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2}) E_0 \cos \theta \delta(r - a) & \text{vanishes upon } \\ \varphi \text{-integration} \\ = 4\pi a^3 \varepsilon_0 (\frac{\varepsilon/\varepsilon_0 - 1}{\varepsilon/\varepsilon_0 + 2}) E_0 \mathbf{e}_z \quad \text{[same as (4.56)]}$$

## 4.7 Electrostatic Energy in Dielectric Media

Let  $\phi(\mathbf{x})$  be the field due to  $\rho_{free}$  and  $\rho_{pol}$  in a dielectric medium. The work done to add  $\delta\rho_{free}$  is

$$\delta W = \int \delta \rho_{free}(\mathbf{x}) \phi(\mathbf{x}) d^3 x$$

$$\delta \rho_{free} = \nabla \cdot \delta \mathbf{D}$$

$$= \int \phi \nabla \cdot \delta \mathbf{D}(\mathbf{x}) d^3 x$$

$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x + \int \mathbf{E} \cdot \delta \mathbf{D} d^3 x$$

$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x + \int \mathbf{E} \cdot \delta \mathbf{D} d^3 x$$

$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x + \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x$$

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$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x$$

$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x + \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x$$

$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x + \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x$$

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$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d^3 x$$

$$= \int \nabla \cdot (\phi \delta \mathbf{D}) d$$

*Note*: (1)  $\rho_{free}(\mathbf{x})$  here is denoted by  $\rho(\mathbf{x})$  in Jackson (4.84).

(2) In a dielectric medium, the addition of  $\delta \rho_{free}(\mathbf{x})$  will induce  $\delta \rho_{pol}(\mathbf{x})$ . Hence,  $\phi(\mathbf{x})$  in the above equation is due to both  $\rho_{free}$  and  $\rho_{pol}$ . The effect of  $\rho_{pol}$  is implicit in  $\mathbf{D}$  (= $\varepsilon \mathbf{E}$ ).

#### 4.7 Electrostatic Energy in Dielectric Media (continued)

$$\delta W = \int \mathbf{E} \cdot \delta \mathbf{D} d^3 x \ [(4.86)] \Rightarrow W = \int d^3 x \int_0^D \mathbf{E} \cdot \delta \mathbf{D}$$
(4.87)

Linear and isotropic media ( $\mathbf{D} = \varepsilon \mathbf{E}$ ;  $\varepsilon$  indep. of  $\mathbf{E}$ ):

$$\mathbf{E} \cdot \delta \mathbf{D} = \mathbf{E} \cdot \delta (\varepsilon \mathbf{E}) = \varepsilon \mathbf{E} \cdot \delta \mathbf{E} = \frac{1}{2} \varepsilon \delta (\mathbf{E} \cdot \mathbf{E}) = \frac{1}{2} \delta (\mathbf{E} \cdot \mathbf{D})$$
Linear and anisotropic media ( $\mathbf{D} = \ddot{\mathbf{E}} \cdot \mathbf{E}$ ;  $\ddot{\mathbf{E}}$  indep. of  $\mathbf{E}$ ):

$$\mathbf{E} \cdot \delta \mathbf{D} = \mathbf{E} \cdot \delta (\ddot{\mathbf{E}} \cdot \mathbf{E}) = \mathbf{E} \cdot \ddot{\mathbf{E}} \cdot \delta \mathbf{E} = \frac{1}{2} \delta (\mathbf{E} \cdot \ddot{\mathbf{E}}) = \frac{1}{2} \delta (\mathbf{E} \cdot \mathbf{D})$$

$$\Rightarrow W = \frac{1}{2} \int d^3 x \int_0^D \delta (\mathbf{E} \cdot \mathbf{D}) = \frac{1}{2} \int \mathbf{E} \cdot \mathbf{D} d^3 x \quad \text{[for linear media]}$$

$$\Rightarrow W = \frac{1}{2} \mathbf{E} \cdot \mathbf{D} \quad \text{[energy/unit volume; for linear media]}$$

$$\mathbf{E} \cdot \mathbf{D} = -\mathbf{D} \cdot \nabla \phi = -\nabla \cdot (\phi \mathbf{D}) + \phi \nabla \cdot \mathbf{D} = -\nabla \cdot (\phi \mathbf{D}) + \rho_{free} \phi$$

$$\Rightarrow W = \frac{1}{2} \int \mathbf{E} \cdot \mathbf{D} d^3 x = \frac{1}{2} \int \rho_{free} (\mathbf{x}) \phi(\mathbf{x}) d^3 x - \frac{1}{2} \oint_S \phi \mathbf{D} \cdot d\mathbf{a}$$

$$= \frac{1}{2} \int \rho_{free} (\mathbf{x}) \phi(\mathbf{x}) d^3 x \quad \text{[for linear media]} \quad \frac{1}{r} \frac{1}{r^2} r^2$$
(14)

$$W = \frac{1}{2} \int \rho_{free} (\mathbf{x}) \phi(\mathbf{x}) d^3 x \quad \text{[(14)]}; \phi \text{ is due to } \rho_{free} & \rho_{pol}.$$
Note:

$$W = \frac{1}{2} \int \rho(\mathbf{x}) \phi(\mathbf{x}) d^3 x \quad \text{[(1.53)]}; \phi \text{ is due to } \rho \text{ in intergrand.}$$

$$W = \int \rho(\mathbf{x}) \phi(\mathbf{x}) d^3 x \quad \text{[(4.24)]}; \phi \text{ is due to external charges.}$$

#### 4.7 Electrostatic Energy in Dielectric Media (continued)

Energy change due to a dielectric object with linear  $\varepsilon_1(\mathbf{x})$  in  $\mathbf{E}_0$  of a fixed external source. (This and next page will not be covered.)

Without the object:  

$$W_{0} = \frac{1}{2} \int \mathbf{E}_{0} \cdot \mathbf{D}_{0} d^{3}x$$
With the object:  

$$W_{1} = \frac{1}{2} \int \mathbf{E} \cdot \mathbf{D} d^{3}x \qquad \mathbf{E}_{0}(\mathbf{x}), \ \mathbf{D}_{0}(\mathbf{x}), \ \phi_{0}(\mathbf{x}) \qquad \mathbf{E}(\mathbf{x}), \ \mathbf{D}(\mathbf{x}), \ \phi(\mathbf{x})$$

$$\Rightarrow \Delta W = W_{1} - W_{0} = \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D} - \mathbf{E}_{0} \cdot \mathbf{D}_{0}) d^{3}x$$

$$= \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_{0} - \mathbf{D} \cdot \mathbf{E}_{0}) d^{3}x + \frac{1}{2} \int (\mathbf{E} + \mathbf{E}_{0}) \cdot (\mathbf{D} - \mathbf{D}_{0}) d^{3}x$$

$$= \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_{0} - \mathbf{D} \cdot \mathbf{E}_{0}) d^{3}x$$

$$= \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_{0} - \mathbf{D} \cdot \mathbf{E}_{0}) d^{3}x$$

$$= \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_{0} - \mathbf{D} \cdot \mathbf{E}_{0}) d^{3}x$$

$$= \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_{0} - \mathbf{D} \cdot \mathbf{E}_{0}) d^{3}x$$

$$= \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_{0} - \mathbf{D} \cdot \mathbf{E}_{0}) d^{3}x = \int (\phi + \phi_{0}) \nabla \cdot (\mathbf{D} - \mathbf{D}_{0}) d^{3}x = 0$$
integration by parts
$$= \rho_{free} - \rho_{free} = 0$$

Reason for  $\nabla \cdot \mathbf{D}_0 = \nabla \cdot \mathbf{D} = \rho_{free}$ : A dielectric object contains no  $\rho_{free}$  and the external source is fixed.  $\Rightarrow \rho_{free}$  is unchanged before and after the introduction of the object.

#### 4.7 Electrostatic Energy in Dielectric Media (continued)

$$\Delta W = \frac{1}{2} \int (\mathbf{E} \cdot \mathbf{D}_0 - \mathbf{D} \cdot \mathbf{E}_0) d^3 x$$

$$\Rightarrow \Delta W \text{ (outside the object)} = 0$$

$$\Rightarrow \Delta W = -\frac{1}{2} \int_{v_1} (\varepsilon_1 - \varepsilon_0) \mathbf{E} \cdot \mathbf{E}_0 d^3 x$$
Outside the object:  $\mathbf{D} = \varepsilon_0 \mathbf{E}$ 
Inside the object:  $\mathbf{D} = \varepsilon_1 \mathbf{E}$ 

$$v_1 \text{ is the volume of the object.}$$

$$v_1 \text{ is the volume of the object.}$$

$$v_2 \text{ is the volume of the object.}$$

$$v_3 \text{ of the object.}$$

 $\Rightarrow$  The dielectric object tends to move toward (away from) the region of increasing  $\mathbf{E}_0$  if  $\varepsilon_1 > \varepsilon_0$  ( $\varepsilon_1 < \varepsilon_0$ ).

$$\mathbf{D} = \varepsilon_1 \mathbf{E} \quad \& \quad \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \quad \Rightarrow \mathbf{P} = (\varepsilon_1 - \varepsilon_0) \mathbf{E}$$

$$\Rightarrow \Delta W = -\frac{1}{2} \int_{\nu_1} \mathbf{P} \cdot \mathbf{E}_0 d^3 x \qquad \text{induced polarization of the object}$$

$$(4.93)$$

 $\Rightarrow$  The energy density of a dielectric object placed in the field  $\mathbf{E}_0$  of a fixed external source is

$$w = -\frac{1}{2} \mathbf{P} \cdot \mathbf{E}_0 \tag{4.94}$$

Question: Explain the factor  $\frac{1}{2}$  which is in (4.94) but not in the 2nd

term of 
$$W = q\phi(0) - \mathbf{p} \cdot \mathbf{E}(0) - \frac{1}{6} \sum_{ij} Q_{ij} \frac{\partial E_j(0)}{\partial x_i} + \cdots$$
 [(4.24)]

## **Appendix A. Taylor Expansion**

Define  $e^{\mathbf{a} \cdot \nabla} = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{a} \cdot \nabla)^n$  [a translational operator]

Taylor expansion of  $f(\mathbf{x} + \mathbf{a})$  and  $\mathbf{A}(\mathbf{x} + \mathbf{a})$  about point  $\mathbf{x}$ :

$$f(\mathbf{x} + \mathbf{a}) = e^{\mathbf{a} \cdot \nabla} f(\mathbf{x}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{a} \cdot \nabla)^n f(\mathbf{x})$$

$$= f(\mathbf{x}) + (\mathbf{a} \cdot \nabla) f(\mathbf{x}) + \frac{1}{2} (\mathbf{a} \cdot \nabla) (\mathbf{a} \cdot \nabla) f(\mathbf{x}) + \cdots$$

$$\mathbf{A}(\mathbf{x} + \mathbf{a}) = e^{\mathbf{a} \cdot \nabla} \mathbf{A}(\mathbf{x}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\mathbf{a} \cdot \nabla)^n \mathbf{A}(\mathbf{x}) \quad \text{derivatives}$$

$$= \mathbf{A}(\mathbf{x}) + (\mathbf{a} \cdot \nabla) \mathbf{A}(\mathbf{x}) + \frac{1}{2} (\mathbf{a} \cdot \nabla) (\mathbf{a} \cdot \nabla) \mathbf{A}(\mathbf{x}) + \cdots$$
(A.1)

Similarly, operating  $f(\mathbf{x})$  and  $\mathbf{A}(\mathbf{x})$  with  $e^{(\mathbf{x}-\mathbf{a})\cdot\nabla}$ , we obtain the Taylor expansion of  $f(\mathbf{x})$  and  $\mathbf{A}(\mathbf{x})$  about point  $\mathbf{a}$ :

$$\begin{cases} f(\mathbf{x}) = f(\mathbf{a}) + \left[ (\mathbf{x} - \mathbf{a}) \cdot \nabla \right] f(\mathbf{a}) + \frac{1}{2} \left[ (\mathbf{x} - \mathbf{a}) \cdot \nabla \right] \left[ (\mathbf{x} - \mathbf{a}) \cdot \nabla \right] f(\mathbf{a}) + \cdots \text{ (A.3)} \\ \mathbf{A}(\mathbf{x}) = \mathbf{A}(\mathbf{a}) + \left[ (\mathbf{x} - \mathbf{a}) \cdot \nabla \right] \mathbf{A}(\mathbf{a}) + \frac{1}{2} \left[ (\mathbf{x} - \mathbf{a}) \cdot \nabla \right] \left[ (\mathbf{x} - \mathbf{a}) \cdot \nabla \right] \mathbf{A}(\mathbf{a}) + \cdots \text{ (A.4)} \\ \text{derivatives evaluated at } \mathbf{a} \end{cases}$$

#### Appendix A. Taylor Expansion (continued)

In (A.1) and (A.2), we have [in Cartesian coordinates]

$$\mathbf{a} \cdot \nabla = a_1 \frac{\partial}{\partial x_1} + a_2 \frac{\partial}{\partial x_2} + a_3 \frac{\partial}{\partial x_3} = \sum_{i=1}^3 a_i \frac{\partial}{\partial x_i}$$
 (A.5)

$$(\mathbf{a} \cdot \nabla)(\mathbf{a} \cdot \nabla) = \sum_{i} a_{i} \frac{\partial}{\partial x_{i}} \sum_{j} a_{j} \frac{\partial}{\partial x_{j}} = \sum_{ij} a_{i} a_{j} \frac{\partial^{2}}{\partial x_{i} \partial x_{j}}$$
(A.6)

$$\left(\mathbf{a} \cdot \nabla\right) f(\mathbf{x}) = \sum_{i} a_{i} \frac{\partial}{\partial x_{i}} f(\mathbf{x}) = \mathbf{a} \cdot \nabla f(\mathbf{x})$$
(A.7)

$$(\mathbf{a} \cdot \nabla) \mathbf{A}(\mathbf{x}) = \sum_{i} a_{i} \frac{\partial}{\partial x_{i}} \left( \sum_{j} A_{j} \mathbf{e}_{j} \right) = \sum_{j} \left( \sum_{i} a_{i} \frac{\partial}{\partial x_{i}} A_{j} \right) \mathbf{e}_{j}$$
(A.8)

Example: 
$$(\mathbf{a} \cdot \nabla)(\mathbf{x} - \mathbf{x}') = \sum_{j} \left[\sum_{i} a_{i} \underbrace{\frac{\partial}{\partial x_{i}}(x_{j} - x'_{j})}_{\delta_{ij}}\right] \mathbf{e}_{j} = \sum_{j} a_{j} \mathbf{e}_{j} = \mathbf{a}$$

For scalar functions with a scalar argument, (A.1) & (A.3) reduce to

$$f(x+a) = f(x) + af'(x) + \frac{1}{2}a^2f''(x) + \cdots$$
 (A.9)

$$f(x) = f(a) + (x - a)f'(a) + \frac{1}{2}(x - a)^2 f''(a) + \cdots$$
 (A.10)

# **Appendix B. Polarization Current Density and** Polarization Charge Density in Dielectric Media

We divide the bound charges (electrons and ions) in a dielectric into different groups. The *i*-th group has  $N_i$  identical charged particles per unit volume. Each particle in the group carries a charge  $e_i$  and has a dipole moment given by  $\mathbf{p}_i = e_i \mathbf{x}_i$ , where  $\mathbf{x}_i$  is the particle's displacement from its equilibrium position under the influence of a static or time-dependent electric field. We assume that the variation of  $\mathbf{x}_i$  of all particles is so small that it will not change  $N_i$ . Then, the electric polarization **P** as a function of position and time can be written as

charge density of the *i*-th group 
$$\mathbf{P}(\mathbf{x},t) = \sum_{i} N_{i}(\mathbf{x})\mathbf{p}_{i}(t) = \sum_{i} N_{i}(\mathbf{x})e_{i}\mathbf{x}_{i}(t) = \sum_{i} \overbrace{\rho_{i}(\mathbf{x})}\mathbf{x}_{i}(t)$$

and the polarization current density is the time derivative of P(x,t)polarization current density

$$\frac{\partial}{\partial t} \mathbf{P}(\mathbf{x}, t) = \sum_{i} \rho_{i}(\mathbf{x}) \frac{d}{dt} \mathbf{x}_{i}(t) = \sum_{i} \rho_{i}(\mathbf{x}) \mathbf{v}_{i}(t) = \mathbf{J}_{pol}(\mathbf{x}, t)$$
(B.1)

#### Appendix B. Polarization Current Density and Polarization Charge Density... (continued)

Let  $\rho_{nol}$  be the polarization charge density of the medium, then

$$\frac{\partial}{\partial t} \rho_{pol} + \nabla \cdot \mathbf{J}_{pol} = 0 \qquad \text{(conservation of charge)}$$

$$\Rightarrow \frac{\partial}{\partial t} \rho_{pol} + \nabla \cdot \frac{\partial}{\partial t} \mathbf{P} = 0 \Rightarrow \frac{\partial}{\partial t} \left( \rho_{pol} + \nabla \cdot \mathbf{P} \right) = 0$$

$$\Rightarrow \rho_{pol} + \nabla \cdot \mathbf{P} = K$$

If P = 0, we have  $\rho_{pol} = 0$ . Hence, K = 0.

$$\Rightarrow \rho_{nol} = -\nabla \cdot \mathbf{P} \tag{B.2}$$

 $\mathbf{J}_{pol}$  is due to the *motion* of bound charges, whereas  $\rho_{pol}$  is due to the displacement of bound charges. The presence of  $\mathbf{J}_{pol}$  does not necessarily imply the presence of  $\rho_{pol}$ , and vice versa. For example, in a static electric field **E**, we have  $\mathbf{J}_{pol} = 0$  because bound charges are stationary. But the stationary charges will be displaced by E; hence  $\rho_{pol} \neq 0$  if  $\nabla \cdot \mathbf{P} \neq 0$ . In time-dependent cases, there must be a  $\mathbf{J}_{pol}$  if  $\mathbf{P} \neq 0$  [hence  $\frac{\partial}{\partial t} \mathbf{P}(\mathbf{x}, t) \neq 0$ ] but not necessarily a  $\rho_{pol}$  unless  $\nabla \cdot \mathbf{P} \neq 0$ .