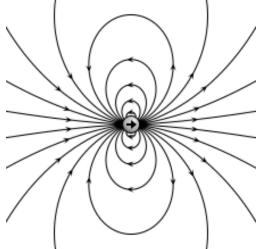
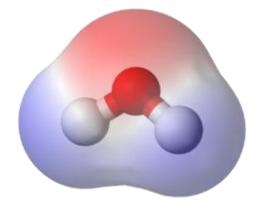
Quantum Mechanics_electric dipole moment

In <u>physics</u>, the **electric dipole moment** is a measure of the separation of positive and negative electrical charges in a system of <u>electric charges</u>, that is, a measure of the charge system's overall <u>polarity</u>. The <u>SI units</u> are <u>Coulomb</u>-meter (C m). This article is limited to static phenomena, and does not describe time-dependent or dynamic polarization.

Elementary definition



Animation showing the <u>Electric field</u> of an electric dipole. The dipole consists of two point electric charges of opposite polarity located close together. A transformation from a point-shaped dipole to a finite-size electric dipole is shown.



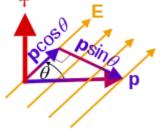
A <u>molecule of water</u> is polar because of the unequal sharing of its electrons in a "bent" structure. A separation of charge is present with negative charge in the middle (red shade), and positive charge at the ends (blue shade).

In the simple case of two point charges, one with charge +q and the other one with charge -q, the electric dipole moment **p** is:

$$\mathbf{p} = q\mathbf{d}$$

where **d** is the <u>displacement vector</u> pointing from the negative charge to the positive charge. Thus, the electric dipole moment vector **p** points from the negative charge to the positive charge. An idealization of this two-charge system is the electrical point dipole consisting of two (infinite) charges only infinitesimally separated, but with a finite **p**.

Torque



Electric dipole **p** and its torque τ in a uniform **E** field.

An object with an electric dipole moment is subject to a <u>torque</u> τ when placed in an external electric field. The torque tends to align the dipole with the field, and makes alignment an orientation of lower <u>potential energy</u> than misalignment. For a spatially uniform electric field **E**, the torque is given by:[1]

$$\boldsymbol{\tau} = \mathbf{p} \times \mathbf{E}$$
,

where **p** is the dipole moment, and the symbol " \times " refers to the <u>vector cross product</u>. The field vector and the dipole vector define a plane, and the torque is directed normal to that plane with the direction given by the <u>right-hand rule</u>.

Expression (general case)

More generally, for a continuous distribution of charge confined to a volume V, the corresponding expression for the dipole moment is:

$$\mathbf{p}(\mathbf{r}) = \int_{V} \rho(\mathbf{r}_0) \left(\mathbf{r}_0 - \mathbf{r}\right) \, d^3 \mathbf{r}_0,$$

where **r** locates the point of observation and $d^3\mathbf{r}_0$ denotes an elementary volume in *V*. For an array of point charges, the charge density becomes a sum of <u>Dirac delta</u> <u>functions</u>:

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} q_i \delta(\mathbf{r} - \mathbf{r}_i),$$

where each \mathbf{r}_i is a vector from some reference point to the charge q_i . Substitution into the above integration formula provides:

$$\mathbf{p}(\mathbf{r}) = \sum_{i=1}^{N} q_i \int_{V} \delta(\mathbf{r}_0 - \mathbf{r}_i) \left(\mathbf{r}_0 - \mathbf{r}\right) d^3 \mathbf{r}_0 = \sum_{i=1}^{N} q_i (\mathbf{r}_i - \mathbf{r}).$$

This expression is equivalent to the previous expression in the case of charge neutrality and N = 2. For two opposite charges, denoting the location of the positive charge of the pair as \mathbf{r}_+ and the location of the negative charge as \mathbf{r}_- :

 $\mathbf{p}(\mathbf{r})$

 $= q_1(\mathbf{r}_1 - \mathbf{r}) + q_2(\mathbf{r}_2 - \mathbf{r}) = q(\mathbf{r}_+ - \mathbf{r}) - q(\mathbf{r}_- - \mathbf{r}) = q(\mathbf{r}_+ - \mathbf{r}_-) = q\mathbf{d},$

showing that the dipole moment vector is directed from the negative charge to the positive charge because the <u>position vector</u> of a point is directed outward from the origin to that point.

The dipole moment is most easily understood when the system has an overall neutral charge; for example, a pair of opposite charges, or a neutral conductor in a uniform electric field. For a system of charges with no net charge, visualized as an array of paired opposite charges, the relation for electric dipole moment is:

$$\mathbf{p}(\mathbf{r}) = \sum_{i=1}^{N} \int_{V} q_{i} [\delta(\mathbf{r_{0}} - (\mathbf{r}_{i} + \mathbf{d}_{i})) - \delta(\mathbf{r_{0}} - \mathbf{r}_{i})] (\mathbf{r}_{0} - \mathbf{r}) d^{3}\mathbf{r}_{0}$$
$$= \sum_{i=1}^{N} q_{i} [\mathbf{r}_{i} + \mathbf{d}_{i} - \mathbf{r} - (\mathbf{r}_{i} - \mathbf{r})]$$
$$= \sum_{i=1}^{N} q_{i} \mathbf{d}_{i} = \sum_{i=1}^{N} \mathbf{p}_{i} ,$$

which is the <u>vector sum</u> of the individual dipole moments of the neutral charge pairs. (Because of overall charge neutrality, the dipole moment is independent of the observer's position \mathbf{r} .) Thus, the value of \mathbf{p} is independent of the choice of reference point, provided the overall charge of the system is zero.

When discussing the dipole moment of a non-neutral system, such as the dipole moment of the <u>proton</u>, a dependence on the choice of reference point arises. In such cases it is conventional to choose the reference point to be the <u>center of mass</u>of the

system, not some arbitrary origin.^[2] It might seem that the center of charge is a more reasonable reference point than the center of mass, but it is clear that this results in a zero dipole moment. This convention ensures that the dipole moment is an <u>intrinsic property</u> of the system.

Potential and field of an electric dipole



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An electric dipole potential map. In blue negative potentials while in red positive ones. An ideal dipole consists of two opposite charges with infinitesimal separation. The potential and field of such an ideal dipole are found next as a limiting case of an example of two opposite charges at non-zero separation.

Two closely spaced opposite charges have a potential of the form:

$$\phi(\mathbf{r}) = \frac{q}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}_+|} - \frac{q}{4\pi\varepsilon_0|\mathbf{r} - \mathbf{r}_-|}$$

with charge separation, d, defined as

 $\mathbf{d} = \mathbf{r}_+ - \mathbf{r}_- \; ,$

The position relative to their center of mass (assuming equal masses), \mathbf{R} , and the unit vector in the direction of \mathbf{R} are given by:

$$\mathbf{R} = \mathbf{r} - \frac{\mathbf{r}_+ + \mathbf{r}_-}{2}, \quad \hat{\mathbf{R}} = \frac{\mathbf{R}}{R}$$

Taylor expansion in d/R (see <u>multipole expansion</u> and <u>quadrupole</u>) allows this potential to be expressed as a series.[3][4]

$$\phi(\mathbf{R}) = \frac{1}{4\pi\varepsilon_0} \frac{q\mathbf{d}\cdot\hat{\mathbf{R}}}{R^2} + O\left(\frac{d^2}{R^2}\right) \approx \frac{1}{4\pi\varepsilon_0} \frac{\mathbf{p}\cdot\hat{\mathbf{R}}}{R^2} \ ,$$

where higher order terms in the series are vanishing at large distances, R, compared to d.[5] Here, the electric dipole moment **p** is, as above:

$$\mathbf{p} = q\mathbf{d}$$
.

The result for the dipole potential also can be expressed as:[6]

$$\phi(\mathbf{R}) = -\mathbf{p} \cdot \nabla \frac{1}{4\pi\varepsilon_0 R} \; ,$$

which relates the dipole potential to that of a point charge. A key point is that the potential of the dipole falls off faster with distance R than that of the point charge.

The electric field of the dipole is the negative gradient of the potential, leading to:[6]

$$\mathbf{E} = \frac{3\mathbf{p} \cdot \mathbf{R}}{4\pi\varepsilon_0 R^3} \hat{\mathbf{R}} - \frac{\mathbf{p}}{4\pi\varepsilon_0 R^3}$$

Thus, although two closely spaced opposite charges are *not quite* an ideal electric dipole (because their potential at short distances is not that of a dipole), at distances much larger than their separation, their dipole moment **p** appears directly in their potential and field.

As the two charges are brought closer together (d is made smaller), the dipole term in the multipole expansion based on the ratio d/R becomes the only significant term at ever closer distances R, and in the limit of infinitesimal separation the dipole term in this expansion is all that matters. As d is made infinitesimal, however, the dipole charge must be made to increase to hold **p** constant. This limiting process results in a "point dipole".

Dipole moment density and polarization density

The dipole moment of an array of charges,

$$\mathbf{p} = \sum_{i=1}^{n} q_i \mathbf{d_i} \; ,$$

determines the degree of polarity of the array, but for a neutral array it is simply a vector property of the array with no information about the array's absolute location. The dipole moment *density* of the array $\mathbf{p}(\mathbf{r})$ contains both the location of the array and its dipole moment. When it comes time to calculate the electric field in some region containing the array, Maxwell's equations are solved, and the information about the charge array is contained in the *polarization density* $\mathbf{P}(\mathbf{r})$ of Maxwell's equations. Depending upon how fine-grained an assessment of the electric field is required, more or less information about the charge array will have to be expressed by $\mathbf{P}(\mathbf{r})$. As explained below, sometimes it is sufficiently accurate to take $\mathbf{P}(\mathbf{r}) = \mathbf{p}(\mathbf{r})$. Sometimes a more detailed description is needed (for example, supplementing the dipole moment density with an additional quadrupole density) and sometimes even more elaborate versions of $\mathbf{P}(\mathbf{r})$ are necessary.

It now is explored just in what way the polarization density $P(\mathbf{r})$ that enters<u>Maxwell's</u> <u>equations</u> is related to the dipole moment \mathbf{p} of an overall neutral array of charges, and also to the *dipole moment density* $\mathbf{p}(\mathbf{r})$ (which describes not only the dipole moment, but also the array location). Only static situations are considered in what follows, so P(r) has no time dependence, and there is no<u>Displacement current</u>. First is some discussion of the polarization density P(r). That discussion is followed with several particular examples.

A formulation of <u>Maxwell's equations</u> based upon division of charges and currents into "free" and "bound" charges and currents leads to introduction of the **D**- and**P**-fields:

 $\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \ ,$

where **P** is called the <u>Polarization density</u>. In this formulation, the divergence of this equation yields:

 $\nabla \cdot \mathbf{D} = \rho_f = \varepsilon_0 \nabla \cdot \mathbf{E} + \nabla \cdot \mathbf{P} \ ,$

and as the divergence term in **E** is the *total* charge, and ρ_f is "free charge", we are left with the relation:

$$\nabla \cdot \mathbf{P} = -\rho_b \; , \;$$

with ρ_b as the bound charge, by which is meant the difference between the total and the free charge densities.

As an aside, in the absence of magnetic effects, Maxwell's equations specify that

 $\nabla \times \mathbf{E} = \mathbf{0}$,

which implies

 $\nabla \times (\mathbf{D} - \mathbf{P}) = \mathbf{0} \; ,$

Applying <u>Helmholtz decomposition</u>:[7]

 $\mathbf{D}-\mathbf{P}=-\nabla\varphi\;,$

for some scalar potential ϕ , and:

 $\nabla \cdot (\mathbf{D} - \mathbf{P}) = \varepsilon_0 \nabla \cdot \mathbf{E} = \rho_f + \rho_b = -\nabla^2 \varphi \; .$

Suppose the charges are divided into free and bound, and the potential is divided into $\varphi=\varphi_f+\varphi_b$.

Satisfaction of the boundary conditions upon ϕ may be divided arbitrarily between ϕ_f and ϕ_b because only the sum ϕ must satisfy these conditions. It follows that **P** is simply proportional to the electric field due to the charges selected as bound, with boundary conditions that prove convenient.[8][9] In particular, when *no* free charge is present, one possible choice is **P** = ϵ_0 **E**.

Next is discussed how several different dipole-moment descriptions of a medium relate to the polarization entering Maxwell's equations.

Medium with charge and dipole densities

As described next, a model for polarization moment density $\mathbf{p}(\mathbf{r})$ results in a polarization

$$\mathbf{P}(\mathbf{r}) = \mathbf{p}(\mathbf{r})$$

restricted to the same model. For a smoothly varying dipole moment distribution**p**(**r**), the corresponding bound charge density is simply

$$\nabla \cdot \mathbf{p}(\mathbf{r}) = \rho_b,$$

as we will establish shortly via integration by parts. However, if $\mathbf{p}(\mathbf{r})$ exhibits an abrupt step in dipole moment at a boundary between two regions, $\nabla \cdot \mathbf{p}(\mathbf{r})$ results in a surface charge component of bound charge. This surface charge can be treated through a surface integral, or by using discontinuity conditions at the boundary, as illustrated in the various examples below.

As a first example relating dipole moment to polarization, consider a medium made up of a continuous charge density $\rho(\mathbf{r})$ and a continuous dipole moment distribution $\mathbf{p}(\mathbf{r})$.[10] The potential at a position \mathbf{r} is:[11][12]

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}_0)}{|\mathbf{r} - \mathbf{r}_0|} d^3 \mathbf{r}_0 + \frac{1}{4\pi\varepsilon_0} \int \frac{\mathbf{p}(\mathbf{r}_0) \cdot (\mathbf{r} - \mathbf{r}_0)}{|\mathbf{r} - \mathbf{r}_0|^3} d^3 \mathbf{r}_0,$$

where $\rho(\mathbf{r})$ is the unpaired charge density, and $\mathbf{p}(\mathbf{r})$ is the dipole moment density.[13] Using an identity:

$$\nabla_{\mathbf{r}_0} \frac{1}{|\mathbf{r} - \mathbf{r}_0|} = \frac{\mathbf{r} - \mathbf{r}_0}{|\mathbf{r} - \mathbf{r}_0|^3}$$

the polarization integral can be transformed:

$$\frac{1}{4\pi\varepsilon_0}\int \frac{\mathbf{p}(\mathbf{r}_0)\cdot(\mathbf{r}-\mathbf{r}_0)}{|\mathbf{r}-\mathbf{r}_0|^3}d^3\mathbf{r}_0 = \frac{1}{4\pi\varepsilon_0}\int \mathbf{p}(\mathbf{r}_0)\cdot\nabla_{\mathbf{r}_0}\frac{1}{|\mathbf{r}-\mathbf{r}_0|}d^3\mathbf{r}_0,$$

= $\frac{1}{4\pi\varepsilon_0}\int \nabla_{\mathbf{r}_0}\cdot\left(\mathbf{p}(\mathbf{r}_0)\frac{1}{|\mathbf{r}-\mathbf{r}_0|}\right)d^3\mathbf{r}_0 - \frac{1}{4\pi\varepsilon_0}\int \frac{\nabla_{\mathbf{r}_0}\cdot\mathbf{p}(\mathbf{r}_0)}{|\mathbf{r}-\mathbf{r}_0|}d^3\mathbf{r}_0,$

The first term can be transformed to an integral over the surface bounding the volume of integration, and contributes a surface charge density, discussed later. Putting this result back into the potential, and ignoring the surface charge for now:

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{r}_0) - \nabla_{\mathbf{r}_0} \cdot \mathbf{p}(\mathbf{r}_0)}{|\mathbf{r} - \mathbf{r}_0|} d^3 \mathbf{r}_0 ,$$

where the volume integration extends only up to the bounding surface, and does not include this surface.

The potential is determined by the total charge, which the above shows consists of:

$$\rho_{\text{total}}(\mathbf{r}_0) = \rho(\mathbf{r}_0) - \nabla_{\mathbf{r}_0} \cdot \mathbf{p}(\mathbf{r}_0) ,$$

showing that:

 $-\nabla_{\mathbf{r}_0} \cdot \mathbf{p}(\mathbf{r}_0) = \rho_b$.

In short, the dipole moment density $\mathbf{p}(\mathbf{r})$ plays the role of the polarization density \mathbf{P} for this medium. Notice, $\mathbf{p}(\mathbf{r})$ has a non-zero divergence equal to the bound charge density (as modeled in this approximation).

It may be noted that this approach can be extended to include all the multipoles: dipole, quadrupole, etc.[14][15] Using the relation:

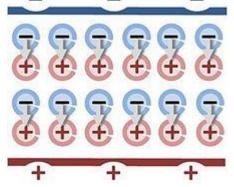
$$\nabla \cdot \mathbf{D} = \rho_f \; ,$$

the polarization density is found to be:

$$\mathbf{P}(\mathbf{r}) = \mathbf{p}_{\mathrm{dip}} - \nabla \cdot \mathbf{p}_{\mathrm{quad}} + \dots ,$$

where the added terms are meant to indicate contributions from higher multipoles. Evidently, inclusion of higher multipoles signifies that the polarization density **P** no longer is determined by a dipole moment density **p**alone. For example, in considering scattering from a charge array, different multipoles scatter an electromagnetic wave differently and independently, requiring a representation of the charges that goes beyond the dipole approximation.[16]

Surface charge



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A uniform array of identical dipoles is equivalent to a surface charge.

Above, discussion was deferred for the first term in the expression for the potential due to the dipoles. Integrating the divergence results in a surface charge. The figure at the right provides an intuitive idea of why a surface charge arises. The figure shows a uniform array of identical dipoles between two surfaces. Internally, the heads and tails of dipoles are adjacent and cancel. At the bounding surfaces, however, no cancellation occurs. Instead, on one surface the dipole heads create a positive surface charge, while at the opposite surface the dipole tails create a negative surface charge. These two opposite surface charges create a net electric field in a direction opposite to the direction of the dipoles.

This idea is given mathematical form using the potential expression above. The potential is:

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int \nabla_{\mathbf{r}_0} \cdot \left(\mathbf{p}(\mathbf{r}_0) \frac{1}{|\mathbf{r} - \mathbf{r}_0|} \right) d^3 \mathbf{r}_0 - \frac{1}{4\pi\varepsilon_0} \int \frac{\nabla_{\mathbf{r}_0} \cdot \mathbf{p}(\mathbf{r}_0)}{|\mathbf{r} - \mathbf{r}_0|} d^3 \mathbf{r}_0 \ .$$

Using the <u>divergence theorem</u>, the divergence term transforms into the surface integral:

$$\begin{aligned} &\frac{1}{4\pi\varepsilon_0} \int \nabla_{\mathbf{r}_0} \cdot \left(\mathbf{p}(\mathbf{r}_0) \frac{1}{|\mathbf{r} - \mathbf{r}_0|} \right) d^3 \mathbf{r}_0 \\ &= \frac{1}{4\pi\varepsilon_0} \int \frac{\mathbf{p}(\mathbf{r}_0) \cdot d\mathbf{A_0}}{|\mathbf{r} - \mathbf{r}_0|} \;, \end{aligned}$$

with dA_0 an element of surface area of the volume. In the event that p(r) is a constant, only the surface term survives:

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \int \frac{1}{|\mathbf{r} - \mathbf{r}_0|} \, \mathbf{p} \cdot d\mathbf{A_0} \; ,$$

with dA_0 an elementary area of the surface bounding the charges. In words, the potential due to a constant **p** inside the surface is equivalent to that of a *surface charge*

$$\sigma = \mathbf{p} \cdot d\mathbf{A}$$

which is positive for surface elements with a component in the direction of \mathbf{p} and negative for surface elements pointed oppositely. (Usually the direction of a surface element is taken to be that of the outward normal to the surface at the location of the element.)

If the bounding surface is a sphere, and the point of observation is at the center of this sphere, the integration over the surface of the sphere is zero: the positive and negative surface charge contributions to the potential cancel. If the point of observation is off-center, however, a net potential can result (depending upon the situation) because the positive and negative charges are at different distances from the point of observation.[17] The field due to the surface charge is:

$$\mathbf{E}(\mathbf{r}) = -\frac{1}{4\pi\varepsilon_0} \nabla_{\mathbf{r}} \int \frac{1}{|\mathbf{r} - \mathbf{r}_0|} \, \mathbf{p} \cdot d\mathbf{A_0} \, ,$$

which, at the center of a spherical bounding surface is not zero (the *fields* of negative and positive charges on opposite sides of the center add because both fields point the same way) but is instead :[18]

$$\mathbf{E} = -\frac{\mathbf{p}}{3\varepsilon_0} \; .$$

If we suppose the polarization of the dipoles was induced by an external field, the polarization field opposes the applied field and sometimes is called a*depolarization field*.[19][20] In the case when the polarization is *outside* a spherical cavity, the field in the cavity due to the surrounding dipoles is in the *same*direction as the polarization.[21]

In particular, if the <u>electric susceptibility</u> is introduced through the approximation:

$$\mathbf{p}(\mathbf{r}) = \varepsilon_0 \chi(\mathbf{r}) \mathbf{E}(\mathbf{r}) \; ,$$

where *E*, in this case and in the following, represent the *external field* which induces the polarization.

Then:

$$\nabla \cdot \mathbf{p}(\mathbf{r}) = \nabla \cdot (\chi(\mathbf{r})\varepsilon_0 \mathbf{E}(\mathbf{r})) = -\rho_b$$
.

Whenever $\chi(\mathbf{r})$ is used to model a step discontinuity at the boundary between two regions, the step produces a surface charge layer. For example, integrating along a normal to the bounding surface from a point just interior to one surface to another point just exterior:

$$\varepsilon_0 \hat{\mathbf{n}} \cdot [\chi(\mathbf{r}_+) \mathbf{E}(\mathbf{r}_+) - \chi(\mathbf{r}_-) \mathbf{E}(\mathbf{r}_-)] = \frac{1}{A_n} \int d\Omega_n \ \rho_b = 0 \ ,$$

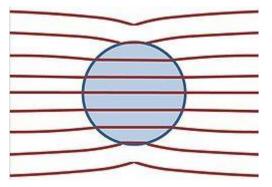
where A_n , Ω_n indicate the area and volume of an elementary region straddling the boundary between the regions, and $\hat{\mathbf{n}}$ a unit normal to the surface. The right side vanishes as the volume shrinks, inasmuch as ρ_b is finite, indicating a discontinuity in *E*, and therefore a surface charge. That is, where the modeled medium includes a step in permittivity, the polarization density corresponding to the dipole moment density

$$\mathbf{p}(\mathbf{r}) = \chi(\mathbf{r})\mathbf{E}(\mathbf{r})$$

necessarily includes the contribution of a surface charge.[22][23][24]

A physically more realistic modeling of $\mathbf{p}(\mathbf{r})$ would have the dipole moment density drop off rapidly, but smoothly to zero at the boundary of the confining region, rather than making a sudden step to zero density. Then the surface charge will not concentrate in an infinitely thin surface, but instead, being the divergence of a smoothly varying dipole moment density, will distribute itself throughout a thin, but finite transition layer.

Dielectric sphere in uniform external electric field



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<u>Field lines</u> of the <u>D-field</u> in a dielectric sphere with greater susceptibility than its surroundings, placed in a previously-uniform field. [25] The <u>Field lines</u> of the <u>E-field</u> (not shown) coincide everywhere with those of the D-field, but inside the sphere, their density is lower, corresponding to the fact that the E-field is weaker inside the sphere than outside. Many of the external E-field lines terminate on the surface of the sphere, where there is a bound charge.

The above general remarks about surface charge are made more concrete by considering the example of a dielectric sphere in a uniform electric field.[26][27]The sphere is found to adopt a surface charge related to the dipole moment of its interior.

A uniform external electric field is supposed to point in the *z*-direction, and spherical-polar coordinates are introduced so the potential created by this field is:

$$\phi_{\infty} = -E_{\infty}z = -E_{\infty}r\cos\theta \; .$$

The sphere is assumed to be described by a <u>dielectric constant</u> κ , that is,

$$\mathbf{D} = \kappa \epsilon_0 \mathbf{E} \; ,$$

and inside the sphere the potential satisfies Laplace's equation. Skipping a few details, the solution inside the sphere is:

$$\phi_{<} = Ar\cos\theta \; ,$$

while outside the sphere:

$$\phi_{>} = \left(Br + \frac{C}{r^2}\right)\cos\theta$$

At large distances, $\phi_{>} \rightarrow \phi_{\infty}$ so $B = -E_{\infty}$. Continuity of potential and of the radial component of displacement $D = \kappa \epsilon_0 E$ determine the other two constants. Supposing the radius of the sphere is R,

$$A = -\frac{3}{\kappa + 2}E_{\infty} ; C = \frac{\kappa - 1}{\kappa + 2}E_{\infty}R^{3} ,$$

As a consequence, the potential is:

$$\phi_{>} = \left(-r + \frac{\kappa - 1}{\kappa + 2} \frac{R^3}{r^2}\right) E_{\infty} \cos\theta ,$$

which is the potential due to applied field and, in addition, a dipole in the direction of the applied field (the *z*-direction) of dipole moment:

$$\mathbf{p} = 4\pi\varepsilon_0 \left(\frac{\kappa - 1}{\kappa + 2}R^3\right) \mathbf{E}_{\infty} ,$$

or, per unit volume:

$$\frac{\mathbf{p}}{V} = 3\varepsilon_0 \left(\frac{\kappa - 1}{\kappa + 2}\right) \mathbf{E}_{\infty} \,.$$

The factor $(\kappa-1)/(\kappa+2)$ is called the <u>Clausius–Mossotti factor</u> and shows that the induced polarization flips sign if $\kappa < 1$. Of course, this cannot happen in this example, but in an example with two different dielectrics κ is replaced by the ratio of the inner to outer region dielectric constants, which can be greater or smaller than one. The potential inside the sphere is:

$$\phi_{<} = -\frac{3}{\kappa+2} E_{\infty} r \cos \theta ,$$

leading to the field inside the sphere:

$$-\nabla\phi_{<} = \frac{3}{\kappa+2}\mathbf{E}_{\infty} = \left(1 - \frac{\kappa-1}{\kappa+2}\right)\mathbf{E}_{\infty} ,$$

showing the depolarizing effect of the dipole. Notice that the field inside the sphere is *uniform* and parallel to the applied field. The dipole moment is uniform throughout the interior of the sphere. The surface charge density on the sphere is the difference between the radial field components:

$$\sigma = 3\varepsilon_0 \frac{\kappa - 1}{\kappa + 2} E_\infty \cos \theta = \frac{1}{V} \mathbf{p} \cdot \hat{\mathbf{R}} .$$

This linear dielectric example shows that the dielectric constant treatment is equivalent to the uniform dipole-moment model and leads to zero charge everywhere except for the surface charge at the boundary of the sphere.

General media

If observation is confined to regions sufficiently remote from a system of charges, a multipole expansion of the exact polarization density can be made. By truncating this expansion (for example, retaining only the dipole terms, or only the dipole and quadrupole terms, or *etc.*), the results of the previous section are regained. In particular, truncating the expansion at the dipole term, the result is indistinguishable

from the polarization density generated by a uniform dipole moment confined to the charge region. To the accuracy of this dipole approximation, as shown in the previous section, the dipole moment *density* $\mathbf{p}(\mathbf{r})$ (which includes not only \mathbf{p} but the location of \mathbf{p}) serves as $\mathbf{P}(\mathbf{r})$.

At locations *inside* the charge array, to connect an array of paired charges to an approximation involving only a dipole moment density **p**(**r**) requires additional considerations. The simplest approximation is to replace the charge array with a model of ideal (infinitesimally spaced) dipoles. In particular, as in the example above that uses a constant dipole moment density confined to a finite region, a surface charge and depolarization field results. A more general version of this model (which allows the polarization to vary with position) is the customary approach using <u>electric susceptibility</u> or <u>electrical permittivity</u>.

A more complex model of the point charge array introduces an <u>effective medium</u>by averaging the microscopic charges;[20] for example, the averaging can arrange that only dipole fields play a role.[28][29] A related approach is to divide the charges into those nearby the point of observation, and those far enough away to allow a multipole expansion. The nearby charges then give rise to *local field effects*.[18][30] In a common model of this type, the distant charges are treated as a homogeneous medium using a dielectric constant, and the nearby charges are treated only in a dipole approximation.[31] The approximation of a medium or an array of charges by only dipoles and their associated dipole moment density is sometimes called the *point dipole* approximation, the <u>discrete dipole approximation</u>, or simply the <u>dipole approximation.[32][33][34]</u>

Dipole moments of fundamental particles

Much experimental work is continuing on measuring the electric dipole moments (EDM) of fundamental and composite particles, namely those of the <u>neutron</u> and<u>electron</u>. As EDMs violate both the <u>Parity</u> (P) and Time (T) symmetries, their values yield a mostly model-independent measure (assuming <u>CPT symmetry</u> is valid) of<u>CP-violation</u> in nature. Therefore, values for these EDMs place strong constraints upon the scale of CP-violation that extensions to the <u>standard model</u> of <u>particle physics</u> may allow.

Indeed, many theories are inconsistent with the current limits and have effectively been ruled out, and established theory permits a much larger value than these limits,

leading to the <u>strong CP problem</u> and prompting searches for new particles such as the <u>axion</u>.

Current generations of experiments are designed to be sensitive to the<u>supersymmetry</u> range of EDMs, providing complementary experiments to those done at the <u>LHC</u>.

Dipole moments of Molecules

<u>Dipole moments in molecules</u> are responsible for the behavior of a substance in the presence of external electric fields. The dipoles tend to be aligned to the external field which can be constant or time-dependent. This effect forms the basis of a modern experimental technique called <u>Dielectric spectroscopy</u>.

Dipole moments can be found in common molecules such as water and also in biomolecules such as proteins.[35]

By means of the total dipole moment of some material one can compute the dielectric constant which is related to the more intuitive concept of conductivity. If \mathcal{M}_{Tot} is the total dipole moment of the sample, then the dielectric constant is given by,

$$\epsilon = 1 + k \langle \mathcal{M}_{\text{Tot}}^2 \rangle$$

where *k* is a constant and $\langle \mathcal{M}_{Tot}^2 \rangle = \langle \mathcal{M}_{Tot}(t=0) \mathcal{M}_{Tot}(t=0) \rangle$ is the time correlation function of the total dipole moment. In general the total dipole moment have contributions coming from translations and rotations of the molecules in the sample,

 $\mathcal{M}_{\mathrm{Tot}} = \mathcal{M}_{\mathrm{Trans}} + \mathcal{M}_{\mathrm{Rot}}.$

Therefore, the dielectric constant (and the conductivity) has contributions from both terms. This approach can be generalized to compute the frequency dependent dielectric function.[36]

The dipole moment of a molecule can also be calculated based on the molecular structure using the concept of group contribution methods.[37]

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- 8. \triangle For example, one could place the boundary around the bound charges at infinity. Then ϕ_b falls off with distance from the bound charges. If an external field is present, and zero free charge, the field can be accounted for in the contribution of ϕ_{f_i} which would arrange to satisfy the boundary conditions and Laplace's equation

 $\nabla^2 \varphi_f = 0 \; .$

- 9. \wedge In principle, one could add the same arbitrary *curl* to both **D** and **P**, which would cancel out of the difference **D P**. However, assuming **D** and **P** originate in a simple division of charges into free and bound, they a formally similar to electric fields and so have zero *curl*.
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