CHAPTER 3 DIPOLE AND QUADRUPOLE MOMENTS

3.1 Introduction



FIGURE III.1

Consider a body which is on the whole electrically neutral, but in which there is a separation of charge such that there is more positive charge at one end and more negative charge at the other. Such a body is an *electric dipole*.

Provided that the body as a whole is electrically neutral, it will experience no *force* if it is placed in a uniform external electric field, but it will (unless very fortuitously oriented) experience a *torque*. The magnitude of the torque depends on its orientation with respect to the field, and there will be two (opposite) directions in which the torque is a *maximum*.

The maximum torque that the dipole experiences when placed in an external electric field is its *dipole moment*. This is a vector quantity, and the torque is a maximum when the dipole moment is at right angles to the electric field. At a general angle, the torque τ , the dipole moment **p** and the electric field **E** are related by

$$\boldsymbol{\tau} = \mathbf{p} \times \mathbf{E}. \tag{3.1.1}$$

The SI units of dipole moment can be expressed as N m $(V/m)^{-1}$. However, work out the dimensions of *p* and you will find that its dimensions are Q L. Therefore it is simpler to express the dipole monent in SI units as coulomb metre, or C m.

Other units that may be encountered for expressing dipole moment are cgs esu, debye, and atomic unit. I have also heard the dipole moment of thunderclouds expressed in kilometre coulombs. A cgs esu is a centimetre-gram-second electrostatic unit. I shall

describe the cgs esu system in a later chapter; suffice it here to say that a cgs esu of dipole moment is about 3.336×10^{-12} C m, and a debye (D) is 10^{-18} cgs esu. An atomic unit of electric dipole moment is a_0e , where a_0 is the radius of the first Bohr orbit for hydrogen and e is the magnitude of the electronic charge. An atomic unit of dipole moment is about 8.478×10^{-29} C m.

I remark in passing that I have heard, distressingly often, some such remark as "The molecule has a dipole". Since this sentence is not English, I do not know what it is intended to mean. It would be English to say that a molecule is a dipole or that it has a dipole moment.

It may be worth spending a little more time on the equation $\tau = \mathbf{p} \times \mathbf{E}$. The equation shows that the resulting torque is, of course, at right angles to the dipole moment vector and to the field. Given, for example, that the dipole moment is $4\mathbf{i} + 3\mathbf{j} + 6\mathbf{k}$ C m, and that the electric field is $2\mathbf{i} + 4\mathbf{j} + 5\mathbf{k}$ N C⁻¹, it is easy to calculate, from the usual rules for a vector product, that the resulting torque is $-9\mathbf{i} - 8\mathbf{j} + 10\mathbf{k}$ N m. It is equally easy to verify, from the usual rules for a scalar product, that the angles between τ and \mathbf{E} and between τ and \mathbf{p} are each 90°. The angle between \mathbf{p} and \mathbf{E} is 17°.

What about the inverse problem? Given that the electric field is **E**, and the torque is τ , what is the dipole moment? One can scarcely say that it is $\frac{\tau}{E}$! In fact, we shall shortly see that the solution is not unique, and shall understand the reason why. Let <u>a</u> solution be \mathbf{p}_0 . Then $\mathbf{p}_0 + \lambda \mathbf{E}$ is also a solution, where λ is any constant having SI units $C^2 N^{-1} m$. (We can see this by substituting $\mathbf{p}_0 + \lambda \mathbf{E}$ for **p** in the equation $\tau = \mathbf{p} \times \mathbf{E}$, and noting that $\mathbf{E} \times \mathbf{E} = \mathbf{0}$.) In effect the component of **p** parallel to **E** is not specified by the equation. Expressed otherwise, the component of a dipole moment parallel to the electric field experiences no torque. Let us then choose \mathbf{p}_0 to be the component of **p** that is perpendicular to **E**. Let us multiply the equation $\tau = \mathbf{p} \times \mathbf{E}$ by $\mathbf{E} \times$, while substituting \mathbf{p}_0 for **p**.

$$\mathbf{E} \times \boldsymbol{\tau} = \mathbf{E} \times (\mathbf{p}_0 \times \mathbf{E}) \qquad 3.1.2$$

On making use of a well-known (!) relation for a triple vector product, namely $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$, we obtain

But $\mathbf{E} \cdot \mathbf{p}_0 = 0$ and

$$\mathbf{E} \times \boldsymbol{\tau} = E^2 \mathbf{p}_0 - (\mathbf{E} \cdot \mathbf{p}_0) \mathbf{E}$$
 3.1.3

so
$$\mathbf{p_0} = \frac{\mathbf{E} \times \mathbf{\tau}}{E^2}$$
 3.1.4

and the general solution is
$$\mathbf{p} = \frac{\mathbf{E} \times \mathbf{\tau}}{\mathbf{E}^2} + \lambda \mathbf{E}.$$
 3.1.5

We can illustrate what this means with a simple drawing, and there is no loss in generality in placing the dipole monent in the plane of the paper and the electric field directed to the right.



It will be agreed that the dipoles labelled \mathbf{p}_0 and $\mathbf{p}_0 + \lambda \mathbf{E}$ will each experience the same torque in the electric field **E**.

Let us return to our numerical example, in which we found that the torque on a dipole was $\tau = -9\mathbf{i} - 8\mathbf{j} + 10\mathbf{k}$ N m when it was placed in an electric field $\mathbf{E} = 2\mathbf{i} + 4\mathbf{j} + 5\mathbf{k}$ N C⁻¹. After a little work, it is found that $\mathbf{p}_0 = \frac{1}{9}(16\mathbf{i} - 13\mathbf{j} + 4\mathbf{k})$ C m. This is the component of **p** perpendicular to the electric field. The general solution is $\mathbf{p} = \frac{1}{9}(16\mathbf{i} - 13\mathbf{j} + 4\mathbf{k}) + \lambda(2\mathbf{i} + 4\mathbf{j} + 5\mathbf{k})$ C m. In our original question, the dipole moment was $4\mathbf{i} + 3\mathbf{j} + 6\mathbf{k}$ C m. Any of the three equations $\frac{16}{9} + 2\lambda = 4$, $-\frac{13}{9} + 4\lambda = 3$, $\frac{4}{9} + 5\lambda = 6$ will result in $\lambda = \frac{10}{9}$ C²N⁻¹ m. In other words, $4\mathbf{i} + 3\mathbf{j} + 6\mathbf{k}$ C m is indeed a possible solution; it is the one for which $\lambda = \frac{10}{9}$ C²N⁻¹ m.

One last small thought before leaving the equation $\tau = \mathbf{p} \times \mathbf{E}$. It may be thought that our derivation of the general solution (equation 3.1.5) is "difficult". After all, who would have thought of applying the operation $\mathbf{E} \times ?$ And who among us remembers the vector identity $\mathbf{A} \times (\mathbf{B} \times \mathbf{C}) = (\mathbf{A} \cdot \mathbf{C})\mathbf{B} - (\mathbf{A} \cdot \mathbf{B})\mathbf{C}$? But a reader with good physical insight might easily arrive at equation 3.1.5 without any need for mathematical legerdemain. Suppose you are asked to solve the equation $\tau = \mathbf{p}_0 \times \mathbf{E}$ given that \mathbf{p} is perpendicular to \mathbf{E} and to τ . This means that \mathbf{p}_0 is in the direction of $\mathbf{E} \times \tau$. And its magnitude must be $\frac{\tau}{E}$, and so the dipole moment in vector form is $\mathbf{p}_0 = \frac{\mathbf{E} \times \tau}{E^2}$. And from physical insight one would understand that, if the dipole moment also had a component in the direction of \mathbf{E} , this would not change the torque on it, and so the general solution must be that given by equation 3.1.5. Sometimes it is easier to solve a problem if you are not very good at mathematics than if you are!

3.2 Mathematical Definition of Dipole Moment

In the introductory section 3.1 we gave a *physical* definition of dipole moment. I am now about to give a *mathematical* definition.



FIGURE III.2

Consider a set of charges Q_1, Q_2, Q_3 ... whose position vectors with respect to a point O are $\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3}$... with respect to some point O. The vector sum

$$\mathbf{p} = \sum Q_i \mathbf{r}_i$$

is the dipole moment of the system of charges with respect to the point O. You can see immediately that the SI unit has to be C m. If we have just a single charge Q whose position vector with respect to O is **r**, the dipole moment of this "system" with respect to O is just Q**r**,

Three important exercises! ...

Exercise. Convince yourself that if the system as a whole is electrically neutral, so that there is as much positive charge as negative charge, the dipole moment so defined is independent of the position of the point O. One can then talk of "the dipole moment of the system" without adding the rider "with respect to the point O".

Exercise. Convince yourself that if any electrically neutral system is placed in an external electric field **E**, it will experience a torque given by $\tau = \mathbf{p} \times \mathbf{E}$, and so the two definitions of dipole moment – the physical and the mathematical – are equivalent.

Exercise. While thinking about these two, also convince yourself (from mathematics or from physics) that the moment of a simple dipole consisting of two charges, +Q and -Q separated by a distance l is Ql. We have already noted that C m is an acceptable SI unit for dipole moment.

3.3 Oscillation of a Dipole in an Electric Field

Consider a dipole oscillating in an electric field (figure III.3). When it is at an angle θ to the field, the magnitude of the restoring torque on it is $pE \sin \theta$, and therefore its equation of motion is $I\ddot{\theta} = -pE\sin\theta$, where *I* is its rotational inertia. For small angles, this is approximately $I\ddot{\theta} = -pE\theta$, and so the period of small oscillations is

$$P = 2\pi \sqrt{\frac{I}{pE}} . \qquad 3.3.1$$

Would you expect the period to be long if the rotational inertia were large? Would you expect the vibrations to be rapid if p and E were large? Is the above expression dimensionally correct?

3.4 Potential Energy of a Dipole in an Electric Field

Refer again to figure III.3. There is a torque on the dipole of magnitude $pE \sin \theta$. In order to increase θ by $\delta\theta$ you would have to do an amount of work $pE \sin \theta \, \delta\theta$. The amount of work you would have to do to increase the angle between **p** and **E** from 0 to θ would be the integral of this from 0 to θ , which is $pE(1 - \cos \theta)$, and this is the potential energy of the dipole, provided one takes the potential energy to be zero when **p** and **E** are parallel. In many applications, writers find it convenient to take the potential energy (P.E.) to be zero when **p** and **E** perpendicular. In that case, the potential energy is

$$P.E. = -pE\cos\theta = -\mathbf{p}\cdot\mathbf{E}. \qquad 3.4.1$$

This is negative when θ is acute and positive when θ is obtuse. You should verify that the product of *p* and *E* does have the dimensions of energy.

3.5 Force on a Dipole in an Inhomogeneous Electric Field

FIGURE III.4

Consider a simple dipole consisting of two charges +Q and -Q separated by a distance δx , so that its dipole moment is $p = Q \,\delta x$. Imagine that it is situated in an inhomogeneous electrical field as shown in figure III.4. We have already noted that a dipole in a *homogeneous* field experiences no net force, but we can see that it *does* experience a net force in an *inhomogeneous* field. Let the field at -Q be E and the field at +Q be $E + \delta E$. The force on -Q is QE to the left, and the force on +Q is $Q(E + \delta E)$ to the right. Thus there is a net force to the right of $Q \,\delta E$, or:

Force =
$$p \frac{dE}{dx}$$
. 3.5.1

Equation 3.5.1 describes the situation where the dipole, the electric field and the gradient are all parallel to the *x*-axis. In a more general situation, all three of these are in different directions. Recall that electric field is minus potential gradient. Potential is a scalar function, whereas electric field is a vector function with three component, of which the *x*-component, for example is $E_x = -\frac{\partial V}{\partial x}$. Field gradient is a symmetric tensor having nine components (of which, however, only six are distinct), such as $\frac{\partial^2 V}{\partial x^2}$, $\frac{\partial^2 V}{\partial y \partial z}$, etc. Thus in general equation 3.5.1 would have to be written as

$$\begin{pmatrix} F_{x} \\ F_{y} \\ F_{z} \end{pmatrix} = - \begin{pmatrix} V_{xx} & V_{xy} & V_{xz} \\ V_{xy} & V_{yy} & V_{yz} \\ V_{xz} & V_{yz} & V_{zz} \end{pmatrix} \begin{pmatrix} p_{x} \\ p_{y} \\ p_{z} \end{pmatrix},$$
 3.5.2

in which the double subscripts in the potential gradient tensor denote the second partial derivatives.

3.6 Induced Dipoles and Polarizability

We noted in section 1.3 that a charged rod will attract an *uncharged* pith ball, and at that time we left this as a little unsolved mystery. What happens is that the rod *induces a dipole moment* in the uncharged pith ball, and the pith ball, which now has a dipole moment, is attracted in the *inhomogeneous field* surrounding the charged rod.

How may a dipole moment be induced in an uncharged body? Well, if the uncharged body is metallic (as in the gold leaf electroscope), it is quite easy. In a metal, there are numerous free electrons, not attached to any particular atoms, and they are free to wander about inside the metal. If a metal is placed in an electric field, the free electrons are attracted to one end of the metal, leaving an excess of positive charge at the other end. Thus a dipole moment is induced.

What about a nonmetal, which doesn't have free electrons unattached to atoms? It may be that the individual molecules in the material have permanent dipole moments. In that case, the imposition of an external electric field will exert a torque on the molecules, and will cause all their dipole moments to line up in the same direction, and thus the bulk material will acquire a dipole moment. The water molecule, for example, has a permanent dipole moment, and these dipoles will align in an external field. This is why pure water has such a large dielectric constant.

But what if the molecules do not have a permanent dipole moment, or what if they do, but they cannot easily rotate (as may well be the case in a solid material)? The bulk material can still become polarized, because a dipole moment is induced in the individual molecules, the electrons inside the molecule tending to be pushed towards one end of the molecule. Or a molecule such as CH₄, which is symmetrical in the absence of an external electric field, may become distorted from its symmetrical shape when placed in an electric field, and thereby acquire a dipole moment.

Thus, one way or another, the imposition of an electric field may induce a dipole moment in most materials, whether they are conductors of electricity or not, or whether or not their molecules have permanent dipole moments.

If two molecules approach each other in a gas, the electrons in one molecule repel the electrons in the other, so that each molecule induces a dipole moment in the other. The two molecules then attract each other, because each dipolar molecule finds itself in the inhomogeneous electric field of the other. This is the origin of the van der Waals forces.

Some bodies (I am thinking about individual molecules in particular, but this is not necessary) are more easily polarized that others by the imposition of an external field. The ratio of the induced dipole moment to the applied field is called the *polarizability* α of the molecule (or whatever body we have in mind). Thus

$$\mathbf{p} = \boldsymbol{\alpha} \mathbf{E}. \qquad 3.6.1$$

The SI unit for α is C m (V m⁻¹)⁻¹ and the dimensions are M⁻¹T²Q².

This brief account, and the general appearance of equation 3.6.1, suggests that \mathbf{p} and \mathbf{E} are in the same direction – but this is so only if the electrical properties of the molecule are isotropic. Perhaps most molecules – and, especially, long organic molecules – have *anisotropic polarizability*. Thus a molecule may be easy to polarize with a field in the *x*-direction, and much less easy in the *y*- or *z*-directions. Thus, in equation 3.6.1, the polarizability is really a symmetric *tensor*, \mathbf{p} and \mathbf{E} are not in general parallel, and the equation, written out in full, is

$$\begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} = \begin{pmatrix} \alpha_{xx} & \alpha_{xy} & \alpha_{xz} \\ \alpha_{xy} & \alpha_{yy} & \alpha_{yz} \\ \alpha_{xz} & \alpha_{yz} & \alpha_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}.$$
3.6.2

(Unlike in equation 3.5.2, the double subscripts are not intended to indicate second partial derivatives; rather they are just the components of the polarizability tensor.) As in several analogous situations in various branches of physics (see, for example, section 2.17 of Classical Mechanics and the inertia tensor) there are three mutually orthogonal directions (the eigenvectors of the polarizability tensor) for which \mathbf{p} and \mathbf{E} will be parallel.

3.7 The Simple Dipole

As you may expect from the title of this section, this will be the most difficult and complicated section of this chapter so far. Our aim will be to calculate the field and potential surrounding a simple dipole.

A simple dipole is a system consisting of two charges, +Q and -Q, separated by a distance 2*L*. The dipole moment of this system is just p = 2QL. We'll suppose that the dipole lies along the *x*-axis, with the negative charge at x = -L and the positive charge at x = +L. See figure III.5.

FIGURE III.5

Let us first calculate the electric field at a point P at a distance y along the y-axis. It will be agreed, I think, that it is directed towards the left and is equal to

$$E_1 \cos \theta + E_2 \cos \theta$$
, where $E_1 = E_2 = \frac{Q}{4\pi\epsilon_0 (L^2 + y^2)}$ and $\cos \theta = \frac{L}{(L^2 + y^2)^{1/2}}$

Therefore
$$E = \frac{2QL}{4\pi\epsilon_0 (L^2 + y^2)^{3/2}} = \frac{p}{4\pi\epsilon_0 (L^2 + y^2)^{3/2}}$$
. 3.7.1

For large *y* this becomes

$$E = \frac{p}{4\pi\varepsilon_0 y^3} \,. \tag{3.7.2}$$

That is, the field falls off as the cube of the distance.

To find the field on the *x*-axis, refer to figure III.6.

FIGURE III.6

It will be agreed, I think, that the field is directed towards the right and is equal to

$$E = E_1 - E_2 = \frac{Q}{4\pi\epsilon_0} \left(\frac{1}{(x-L)^2} - \frac{1}{(x+L)^2} \right).$$
 3.7.3

This can be written $\frac{Q}{4\pi\varepsilon_0 x^2} \left(\frac{1}{(1-L/x)^2} - \frac{1}{(1+L/x)^2} \right)$, and on expansion of this by

the binomial theorem, neglecting terms of order $(L/x)^2$ and smaller, we see that at large x the field is

$$E = \frac{2p}{4\pi\varepsilon_0 x^3} \,. \tag{3.7.4}$$

Now for the field at a point P that is neither on the axis (*x*-axis) nor the equator (*y*-axis) of the dipole. See figure III.7.

FIGURE III.7

It will probably be agreed that it would not be particularly difficult to write down expressions for the contributions to the field at P from each of the two charges in turn. The difficult part then begins; the two contributions to the field are in different and awkward directions, and adding them vectorially is going to be a bit of a headache.

It is much easier to calculate the *potential* at P, since the two contributions to the potential can be added as scalars. Then we can find the x- and y-components of the field by calculating $\partial V/\partial x$ and $\partial V/\partial y$.

Thus
$$V = \frac{Q}{4\pi\varepsilon_0} \left(\frac{1}{\{(x-L)^2 + y^2\}^{1/2}} - \frac{1}{\{(x+L)^2 + y^2\}^{1/2}} \right).$$
 3.7.5

To start with I am going to investigate the potential and the field at a *large distance* from the dipole – though I shall return later to the near vicinity of it.

At *large distances* from a small dipole (see figure III.8), we can write $r^2 = x^2 + y^2$,

FIGURE III.8

and, with $L^2 \ll r^2$, the expression 3.7.5 for the potential at P becomes

$$V = \frac{Q}{4\pi\varepsilon_0} \left(\frac{1}{(r^2 - 2Lx)^{1/2}} - \frac{1}{(r^2 + 2Lx)^{1/2}} \right) = \frac{Q}{4\pi\varepsilon_0 r} \left((1 - 2Lx/r^2)^{-1/2} - (1 + 2Lx/r^2)^{-1/2} \right)$$

When this is expanded by the binomial theorem we find, to order L/r, that the potential can be written in any of the following equivalent ways:

$$V = \frac{2QLx}{4\pi\epsilon_0 r^3} = \frac{px}{4\pi\epsilon_0 r^3} = \frac{p\cos\theta}{4\pi\epsilon_0 r^2} = \frac{\mathbf{p}\cdot\mathbf{r}}{4\pi\epsilon_0 r^3}.$$
 3.7.6

Thus the equipotentials are of the form

$$r^2 = c\cos\theta, \qquad 3.7.7$$

where

$$c = \frac{p}{4\pi\varepsilon_0 V}$$
 3.7.8

Now, bearing in mind that $r^2 = x^2 + y^2$, we can differentiate $V = \frac{px}{4\pi\epsilon_0 r^3}$ with respect to x and y to find the x- and y-components of the field.

Thus we find that

$$E_x = \frac{p}{4\pi\varepsilon_0} \left(\frac{3x^2 - r^2}{r^5}\right) \text{ and } E_y = \frac{pxy}{4\pi\varepsilon_0 r^5}.$$
 3.7.9a,b

We can also use polar coordinates to find the radial and transverse components from $E_r = -\frac{\partial V}{\partial r}$ and $E_{\theta} = -\frac{1}{r}\frac{\partial V}{\partial \theta}$ together with $V = \frac{p\cos\theta}{4\pi\varepsilon_0 r^2}$ to obtain $E_r = \frac{2p\cos\theta}{4\pi\varepsilon_0 r^3}$, $E_{\theta} = \frac{p\sin\theta}{4\pi\varepsilon_0 r^3}$ and $E = \frac{p}{4\pi\varepsilon_0 r^3}\sqrt{1+3\cos^2\theta}$. 3.7.10a,b,c

The angle that **E** makes with the axis of the dipole at the point (r, θ) is $\theta + \tan^{-1} \frac{1}{2} \tan \theta$.

For those who enjoy vector calculus, we can also say $\mathbf{E} = -\frac{1}{4\pi\epsilon_0} \nabla \left(\frac{\mathbf{p} \cdot \mathbf{r}}{r^3}\right)$, from which, after a little algebra and quite a lot of vector calculus, we find

$$\mathbf{E} = \frac{1}{4\pi\varepsilon_0} \left(\frac{3(\mathbf{p} \cdot \mathbf{r})\mathbf{r}}{r^5} - \frac{\mathbf{p}}{r^3} \right).$$
 3.7.11

This equation contains all the information that we are likely to want, but I expect most readers will prefer the more explicit rectangular and polar forms of equations 3.7.9 and 3.7.10.

Equation 3.7.7 gives the equation to the equipotentials. The equation to the lines of force can be found as follows. Referring to figure III.9, we see that the differential equation to the lines of force is

which, upon integration, becomes

$$r = a\sin^2\theta. \qquad 3.7.13$$

Note that the equations $r^2 = c \cos \theta$ (for the equipotentials) and $r = a \sin^2 \theta$ (for the lines of force) are orthogonal trajectories, and either can be derived from the other. Thus, given that the differential equation to the lines of force is $r \frac{d\theta}{dr} = \frac{1}{2} \tan \theta$ with solution $r = a \sin^2 \theta$, the differential equation to the orthogonal trajectories (i.e. the equipotentials) is $-\frac{1}{r} \frac{dr}{d\theta} = \frac{1}{2} \tan \theta$, with solution $r^2 = c \cos \theta$.

In figure III.10, there is supposed to be a tiny dipole situated at the origin. The unit of length is L, half the length of the dipole. I have drawn eight electric field lines (continuous), corresponding to a = 25, 50, 100, 200, 400, 800, 1600, 3200. If r is

expressed in units of L, and if V is expressed in units of $\frac{Q}{4\pi\epsilon_0 L}$, the equations 3.7.7 and

3.7.8 for the equipotentials can be written $r = \sqrt{\frac{2\cos\theta}{V}}$, and I have drawn seven equipotentials (dashed) for V = 0.0001, 0.0002, 0.0004, 0.0008, 0.0016, 0.0032, 0.0064. It will be noticed from equation 3.7.9a, and is also evident from figure III.10, that E_x is zero for $\theta = 54^{\circ}$ 44'.

At the end of this chapter I append a (geophysical) exercise in the geometry of the field at a large distance from a small dipole.

Equipotentials near to the dipole

These, then, are the field lines and equipotentials at a *large distance* from the dipole. We arrived at these equations and graphs by expanding equation 3.7.5 binomially, and neglecting terms of higher order than L/r. We now look *near to* the dipole, where we cannot make such an approximation. Refer to figure III.7.

We can write 3.7.5 as

$$V(x, y) = \frac{Q}{4\pi\epsilon_0} \left(\frac{1}{r_1} - \frac{1}{r_2} \right),$$
 3.7.14

where $r_1^2 = (x - L)^2 + y^2$ and $r_2^2 = (x + L)^2 + y^2$. If, as before, we express distances in terms of *L* and *V* in units of $\frac{Q}{4\pi\epsilon_0 L}$, the expression for the potential becomes

$$V(x, y) = \frac{1}{r_1} - \frac{1}{r_2}, \qquad 3.7.15$$

where $r_1^2 = (x+1)^2 + y^2$ and $r_2^2 = (x-1)^2 + y^2$.

One way to plot the equipotentials would be to calculate V for a whole grid of (x, y) values and then use a contour plotting routine to draw the equipotentials. My computing skills are not up to this, so I'm going to see if we can find some way of plotting the equipotentials directly.

I present two methods. In the first method I use equation 3.7.15 and endeavour to manipulate it so that I can calculate y as a function of x and V. The second method was shown to me by J. Visvanathan of Chennai, India. We'll do both, and then compare them.

First Method.

To anticipate, we are going to need the following:

$$r_1^2 r_2^2 = (x^2 + y^2 + 1)^2 - 4x^2 = B^2 - A,$$
 3.7.16

$$r_1^2 + r_2^2 = 2(x^2 + y^2 + 1) = 2B,$$
 3.7.17

and

$$r_1^4 + r_2^4 = 2[(x^2 + y^2 + 1)^2 + 4x^2] = 2(B^2 + A),$$
 3.7.18

where

$$A = 4x^2 \qquad \qquad 3.7.19$$

and

$$B = x^2 + y^2 + 1. 3.7.20$$

Now equation 3.7.15 is $r_1r_2V = r_2 - r_1$. In order to extract y it is necessary to square this twice, so that r_1 and r_2 appear only as r_1^2 and r_2^2 . After some algebra, we obtain

$$r_1^2 r_2^2 [2 - V^4 r_1^2 r_2^2 + 2V^2 (r_1^2 + r_2^2)] = r_1^4 + r_2^4.$$
 3.7.21

Upon substitution of equations 3.7.16, 17, 18, for which we are well prepared, we find for the equation to the equipotentials an equation which, after some algebra, can be written as a quartic equation in *B*:

$$a_0 + a_1 B + a_2 B^2 + a_3 B^3 + a_4 B^4 = 0, \qquad 3.7.22$$

where

and

$$a_0 = A(4 + V^4 A), 3.7.23$$

$$a_1 = 4V^2 A,$$
 3.7.24

$$a_2 = -2V^2 A,$$
 3.7.25

$$a_3 = -4V^2$$
, 3.7.26

$$a_4 = V^4$$
. 3.7.27

The algorithm will be as follows: For a given V and x, calculate the quartic coefficients from equations 3.7.23-27. Solve the quartic equation 3.7.22 for B. Calculate y from equation 3.7.20. My attempt to do this is shown in figure III.11. The dipole is supposed to have a negative charge at (-1, 0) and a positive charge at (+1, 0). The equipotentials are drawn for V = 0.05, 0.10, 0.20, 0.40, 0.80.

Second method (J. Visvanathan).

In this method, we work in polar coordinates, but instead of using the coordinates (r, θ) , in which the origin, or pole, of the polar coordinate system is at the centre of the dipole (see figure III.7), we use the coordinates (r_1, ϕ) with origin at the positive charge.

From the triangle, we see that

$$r_2^2 = r_1^2 + 4L^2 + 4Lr_1\cos\phi. \qquad 3.7.28$$

For future reference we note that

$$\frac{\partial r_2}{\partial r_1} = \frac{r_1 + 2L\cos\phi}{r_2}.$$
 3.7.29

Provided that distances are expressed in units of L, these equations become

$$r_2^2 = r_1^2 + 4r_1\cos\phi + 4, \qquad 3.7.30$$

$$\frac{\partial r_2}{\partial r_1} = \frac{r_1 + 2\cos\phi}{r_2}.$$
 3.7.31

If, in addition, electrical potential is expressed in units of $\frac{Q}{4\pi\epsilon_0 L}$, the potential at P is given, as before (equation 3.17.15), by

$$V(r_1, \phi) = \frac{1}{r_1} - \frac{1}{r_2}.$$
 3.7.32

Recall that r_2 is given by equation 3.7.30, so that equation 3.7.32 is really an equation in just *V*, r_1 and ϕ .

In order to plot an equipotential, we fix some value of V; then we vary ϕ from 0 to π , and, for each value of ϕ we have to try to calculate r_1 . This can be done by the Newton-Raphson process, in which we make a guess at r_1 and use the Newton-Raphson process to obtain a better guess, and continue until successive guesses converge. It is best if we can make a fairly good first guess, but the Newton-Raphson process will often converge very rapidly even for a poor first guess.

Thus we have to solve the following equation for r_1 for given values of V and ϕ ,

$$f(r_1) = \frac{1}{r_1} - \frac{1}{r_2} - V = 0, \qquad 3.7.33$$

bearing in mind that r_2 is given by equation 3.7.31.

By differentiation with respect to r_1 , we have

$$f'(r_1) = -\frac{1}{r_1^2} + \frac{1}{r_2^2} \frac{\partial r_2}{\partial r_1} = -\frac{1}{r_1^2} + \frac{r_1 + 2\cos\phi}{r_2^3}, \qquad 3.7.34$$

and we are all set to begin a Newton-Raphson iteration: $r_1 = r_1 - f/f'$. Having obtained r_1 , we can then obtain the (x, y) coordinates from $x = 1 + r_1 \cos \phi$ and $y = r_1 \sin \phi$.

I tried this method and I got exactly the same result as by the first method and as shown in figure III.11.

So which method do we prefer? Well, anyone who has worked through in detail the derivations of equations 3.7.16 -3.7.27, and has then tried to program them for a computer, will agree that the first method is very laborious and cumbersome. By comparison Visvanathan's method is much easier both to derive and to program. On the other hand, one small point in favour of the first method is that it involves no trigonometric functions, and so the numerical computation is potentially faster than the second method in which a trigonometric function is calculated at each iteration of the

Newton-Raphson process. In truth, though, a modern computer will perform the calculation by either method apparently instantaneously, so that small advantage is hardly relevant.

So far, we have managed to draw the *equipotentials* near to the dipole. The *lines of force* are orthogonal to the equipotentials. After I tried several methods with only partial success, I am grateful to Dr Visvanathan who pointed out to me what ought to have been the "obvious" method, namely to use equation 3.7.12, which, in our (r_1, ϕ) coordinate

system based on the positive charge, is $r_1 \frac{d\phi}{dr_1} = \frac{E_{\phi}}{E_{r_1}}$, just as we did for the large

distance, small dipole, approximation. In this case, the potential is given by equations 3.7.30 and 3.7.32. (Recall that in these equations, distances are expressed in units of L and the potential in units of $\frac{Q}{4\pi\varepsilon_0 L}$.) The radial and transverse components of the field

are given by $E_{r_1} = -\frac{\partial V}{\partial r_1}$ and $E_{\phi} = -\frac{1}{r_1}\frac{\partial V}{\partial \phi}$, which result in

$$E_{r_1} = \frac{1}{r_1^2} - \frac{r_1 + 2\cos\phi}{r_2^3}$$
 3.7.35

and

$$E_{\phi} = \frac{2\sin\phi}{r_2^3}.$$
 3.7.36

Here, the field is expressed in units of $\frac{Q}{4\pi\epsilon_0 L^2}$, although that hardly matters, since we are interested only in the ratio. On applying $r_1 \frac{d\phi}{dr_1} = \frac{E_{\phi}}{E_r}$ to these field components we

are interested only in the ratio. On applying $r_1 \frac{1}{dr_1} = \frac{1}{E_{r_1}}$ to these field components v obtain the following differential equation to the lines of force:

$$d\phi = \frac{2r_1 \sin \phi}{\left(r_1^2 + 4 + 4r_1 \cos \phi\right)^{3/2} - r_1^2(r_1 + 2\cos \phi)} dr_1.$$
 3.7.37

Thus one can start with some initial ϕ_0 and small r_2 and increase r_1 successively by small increments, calculating a new ϕ each time. The results are shown in figure III.12, in which the equipotentials are drawn for the same values as in figure III.11, and the initial angles for the lines of force are 30°, 60°, 90°, 120°, 150°.

Here's yet another method of calculating the potential near to a dipole, for those who are familiar with Legendre polynomials. For those who are not familiar with them, here's a quick introduction:

The expression $(r^2 + a^2 - 2rx)^{-1/2}$ turns up quite often in various geometrical situations in physics. Unsurprisingly (think of the Cosine Rule in solving a plane triangle) it often turns up in a context where x is of the form $x = a\cos\theta$. That is, we have to deal with an expression of the form $(r^2 + a^2 - 2ar\cos\theta)^{-1/2}$. This can be written $\left[1 + (\frac{a}{r})^2 - 2(\frac{a}{r})\cos\theta\right]^{-1/2}/r$ With an effort (some might say with a considerable effort) this can be expanded by the binomial theorem as a power series in $(\frac{a}{r})$, in which the successive coefficients are functions of (in fact polynomials in) $\cos\theta$. Thus

$$\begin{bmatrix} 1 + (\frac{a}{r})^2 - 2(\frac{a}{r})\cos\theta \end{bmatrix}^{-1/2} = P_0(\cos\theta) + P_1(\cos\theta)(\frac{a}{r}) + P_2(\cos\theta)(\frac{a}{r})^2 + \dots$$

and of course,
$$\begin{bmatrix} 1 + (\frac{a}{r})^2 + 2(\frac{a}{r})\cos\theta \end{bmatrix}^{-1/2} = P_0(\cos\theta) - P_1(\cos\theta)(\frac{a}{r}) + P_2(\cos\theta)(\frac{a}{r})^2 - \dots$$

The first few of these coefficients, which are called Legendre Polynomials, are

 $P_0(\cos \theta) = 1$ $P_1(\cos \theta) = \cos \theta$ $P_2(\cos \theta) = \frac{1}{2}(3\cos^2 \theta - 1)$ $P_3(\cos \theta) = \frac{1}{2}(5\cos^3 \theta - 3\cos \theta)$ $P_4(\cos \theta) = \frac{1}{8}(35\cos^4 - 30\cos^2 \theta + 3)$ $P_5(\cos \theta) = \frac{1}{8}(63\cos^5 - 70\cos^3 \theta + 15\cos \theta)$

Extensive tables of these, as well as other properties of the Legendre polynomials can be found in various places. I list some of them in Section 1.13 of my site www.astro.uvic.ca/~tatum/celmechs/celm1.pdf

Now back to the dipole:

The potential at P is given by

$$4\pi\varepsilon_0 V = Q \left[\frac{1}{(a^2 + r^2 - 2ar\cos\theta)^{1/2}} - \frac{1}{(a^2 + r^2 + 2ar\cos\theta)^{1/2}} \right]$$
$$= \frac{Q}{r} \left[(1 - 2(\frac{a}{r})\cos\theta + (\frac{a}{r})^2)^{-1/2} - (1 + 2(\frac{a}{r})\cos\theta + (\frac{a}{r})^2)^{-1/2} \right].$$

Expand this:

$$4\pi\varepsilon_0 V = \frac{Q}{r} \Big[P_0(\cos\theta) + P_1(\cos\theta)(\frac{a}{r}) + P_2(\cos\theta)(\frac{a}{r})^2 + \dots - [P_0(\cos\theta) - P_1(\cos\theta)(\frac{a}{r}) + P_2(\cos\theta)(\frac{a}{r})^2 - \dots] \Big]$$

$$V = \frac{2Q}{4\pi\varepsilon_0 r} \Big[P_1(\cos\theta)(\frac{a}{r}) + P_3(\cos\theta)(\frac{a}{r})^3 + P_5(\cos\theta)(\frac{a}{r})^5 + \dots \Big].$$
 3.7.38

For large r only the first term contributes appreciably and the expression then becomes

 $V \approx \frac{2Qa\cos\theta}{4\pi\epsilon_0 r^2} = \frac{p\cos\theta}{4\pi\epsilon_0 r^2}$, where p = 2Qa is the dipole moment. For smaller r (closer to

the dipole, we add higher-order terms. We can convert to cartesian components if needed, and we can find the field components by partial differentiation in the appropriate directions.

3.8 A Geophysical Example

Assume that planet Earth is spherical and that it has a little magnet or current loop at its centre. By "little" I mean small compared with the radius of the Earth. Suppose that, at a large distance from the magnet or current loop the geometry of the magnetic field is the same as that of an electric field at a large distance from a simple dipole. That is to say, the equation to the lines of force is $r = a \sin^2 \theta$ (equation 3.7.13), and the differential equation to the lines of force is $\frac{dr}{d\theta} = \frac{2r}{\tan \theta}$ (equation 3.7.12).

Show that the angle of dip D at geomagnetic latitude L is given by

$$\tan D = 2 \tan L. \qquad 3.8.1$$

The geometry is shown in figure III.14.

The result is a simple one, and there is probably a simpler way of getting it than the one I tried. Let me know (jtatum at uvic dot ca) if you find a simpler way. In the meantime, here is my solution.

I am going to try to find the slope m_1 of the tangent to Earth (i.e. of the horizon) and the slope m_2 of the line of force. Then the angle D between them will be given by the equation (which I am hoping is well known from coordinate geometry!)

$$\tan D = \frac{m_1 - m_2}{1 + m_1 m_2}.$$
 3.8.2

The first is easy:

$$m_1 = \tan(90^\circ + \theta) = -\frac{1}{\tan \theta}.$$
 3.8.3

For m_2 we want to find the slope of the line of force, whose equation is given in polar coordinates. So, how do you find the slope of a curve whose equation is given in polar coordinates? We can do it like this:

$$\begin{aligned} x &= r\cos\theta, \\ y &= r\sin\theta, \end{aligned}$$
 3.8.4
3.8.5

$$y = r\sin\theta, \qquad 3.8.5$$

$$dr = \cos\theta dr - r\sin\theta d\theta \qquad 38.6$$

$$dy = \sin\theta dr + r\cos\theta d\theta. \qquad 3.8.7$$

From these, we obtain

$$\frac{dy}{dx} = \frac{\sin\theta \frac{dr}{d\theta} + r\cos\theta}{\cos\theta \frac{dr}{d\theta} - r\sin\theta}.$$
 3.8.8

In our particular case, we have $\frac{dr}{d\theta} = \frac{2r}{\tan\theta}$ (equation 3.7.12), so if we substitute this into equation 3.10.8 we soon obtain

$$m_2 = \frac{3\sin\theta\cos\theta}{3\cos^2\theta - 1}.$$
 3.8.9

Now put equations 3.8.3 and 3.8.9 into equation 3.8.2, and, after a little algebra, we soon obtain

$$\tan D = \frac{2}{\tan \theta} = 2 \tan L.$$
3.8.10

Here is another question. The magnetic field is generally given the symbol B. Show that the strength of the magnetic field B(L) at geomagnetic latitude L is given by

$$B(L) = B(0)\sqrt{1 + 3\sin^2 L},$$
 3.8.11

where B(0) is the strength of the field at the equator. This means that it is twice as strong at the magnetic poles as at the equator.

Start with equation 3.7.2, which gives the electric field at a distant point on the equator of an electric dipole. That equation was $E = \frac{p}{4\pi\epsilon_0 y^3}$. In this case we are dealing with a magnetic field and a magnetic dipole, so we'll replace the electric field *E* with a magnetic field *B*. Also $p/(4\pi\epsilon_0)$ is a combination of electrical quantities, and since we are interested only in the geometry (i.e. on how *B* varies from equation to pole, let's just write $p/(4\pi\epsilon_0)$ as *k*. And we'll take the radius of Earth to be *R*, so that equation 3.7.2 gives for the magnetic field at the surface of Earth on the equator as

$$B(0) = \frac{k}{R^3}.$$
 3.8.12

In a similar vein, equations 3.7.10a,b for the radial and transverse components of the field at geomagnetic latitude *L* (which is $90^{\circ} - \theta$) become

$$B_r(L) = \frac{2k \sin L}{R^3}$$
 and $B_{\theta}(L) = \frac{k \cos L}{R^3}$. 3.8.13a,b

And since $B = \sqrt{B_r^2 + B_{\theta}^2}$, the result immediately follows.

3.9 Second moments of mass

If we have a collection of point masses, we can calculate a number of second moments. Likewise, if we have a collection of point charges, we can calculate a number of second moments. There are many similarities between the two situations - but there are a few differences. The differences arise partly from tradition, but they mostly arise from the circumstance that there is only one sort of mass, whereas there are two sorts of charges - positive and negative.

In this section we briefly review the concepts of second moments of mass (with which we assume the reader is already familiar). In the next section we introduce second moments of charge, so that the reader can compare and contrast the two.

If we have a collection of point masses - m_1 at (x_1, y_1, z_1) , m_2 at (x_2, y_2, z_2) , etc., we can calculate several second moments. We can calculate the second moments with respect to the y_2 -, z_x - and x_y -planes:

$$\Sigma m_i x_i^2$$
, $\Sigma m_i y_i^2$, $\Sigma m_i z_i^2$

As far as I know these particular moments don't have much of a role in dynamical theory.

We can calculate the second moments with respect to the *x*-, *y*, and *z*-<u>axes</u>. These do play a very large role in dynamical theory, and, physically, they are respectively the rotational inertias about the *x*-, *y*, and *z*-<u>axes</u> - i.e. the ratio of an applied torque to a resultant angular acceleration. They are usually given the symbols *A*, *B* and *C*:

$$A = \sum m_i (y_i^2 + z_i^2), \quad B = \sum m_i (z_i^2 + x_i^2), \quad C = \sum m_i (x_i^2 + y_i^2)$$
 3.9.1

We can calculate the mixed second moments. They, too, play a large role, and are usually given the symbols F, G and H.

$$F = \sum m_i y_i z_i, \quad G = \sum m_i z_i x_i, \quad F = \sum m_i x_i y_i. \quad 3.9.2$$

It is often useful to gather these together in a matrix known as the *inertia tensor*:

$$\mathbf{I} = \begin{pmatrix} A & -H & -G \\ -H & B & -F \\ -G & -F & C \end{pmatrix}$$
 3.9.3

This tensor appears in the relation between the angular momentum L and the angular velocity $\boldsymbol{\omega}$ of a solid body: $\mathbf{L} = \mathbf{I}\boldsymbol{\omega}$.

One further second moment that can be calculated is the second moment about a <u>point</u> (perhaps about the origin of coordinates). I use the symbol \mathcal{I} for this. It is known as the geometric moment of inertia (in contrast to the dynamic moment of inertia), and it is defined by

$$\mathcal{J} = \sum m_i r_1^2 = \sum m_i (x_i^2 + y_i^2 + z_i^2) = \frac{1}{2} (A + B + C) = \frac{1}{2} \operatorname{Tr} \mathbf{I}$$
 3.9.4

With all these second moments available, the term "moment of inertia" is open to some ambiguity, and it may not always be used in different contexts or by different writers to mean exactly the same thing.

When we have system of point masses, it is often convenient to refer to a point $(\bar{x}, \bar{y}, \bar{z})$ known as the *centre of mass* and defined by

$$M\overline{x} = \sum m_i x_i$$
, $M\overline{y} = \sum m_i y_i$, $M\overline{z} = \sum m_i z_i$, 3.9.5

where $M = \sum m_i$.

If instead of a collection of point masses we have a single extended solid body whose density ρ varies from point to point according to $\rho = \rho(x, y, z)$, the various moments are calculated, if we are working in cartesian coordinates, by integrals such as

$$A = \iiint (y^2 + z^2) \rho(x, y, z) dx dy dz \qquad 3.9.6$$

etc. The limits of integration extend from the origin to the surface of the body, or, since the density outside the body is presumably zero, the limits might as well be from 0 to ∞ .

3.10 Second moments of charge

If we have a collection of point charges - Q_1 at (x_1, y_1, z_1) , Q_2 at (x_2, y_2, z_2) , etc., we can calculate several second moments. We can calculate the second moments with respect to the *yz*-, *zx*- and *xy*-planes:

$$\Sigma Q_i x_i^2$$
, $\Sigma Q_i y_i^2$, $\Sigma Q_i z_i^2$. 3.10.1

In contrast to describing a system of point masses, these <u>do</u> play a role in electrostatic theory, and I denote them respectively by q_{xx} , q_{yy} , q_{zz} . Note that I am using the symbol Q_i for electric charge, and symbols such as q_{xx} for elements of what we shall come to know as the *quadrupole moment tensor*.

We can also calculate the second moments with respect to the x-, y, and z-<u>axes:</u>

$$\Sigma Q_i(y_i^2 + z_i^2), \ \Sigma Q_i(z_i^2 + x_i^2), \ \Sigma Q_i(x_i^2 + y_i^2)$$
,

but as far as I know these do not play a significant role in electrostatic theory, so I shan't give them any particular symbols, nor shall I give them with an equation number.

We can calculate the mixed second moments.

$$q_{yz} = \sum Q_i y_i z_i, \quad q_{zx} = \sum Q_i z_i x_i, \quad q_{xy} = \sum Q_i x_i y_i.$$
 3.10.2

It is often useful to gather these together in a matrix known as the *quadrupole moment matrix*.

$$\mathbf{q} = \begin{pmatrix} q_{xx} & q_{xy} & q_{zx} \\ q_{xy} & q_{yy} & q_{yz} \\ q_{zx} & q_{yz} & q_{zz} \end{pmatrix}$$
3.10.3

This is a symmetric matrix, because q_{xy} is obviously the same as q_{yx} . I have chosen to write the subscripts in cyclic order in each of these matrix elements, regardless of row or column.

One further second moment that can be calculated is the second moment about a <u>point</u> (perhaps about the origin of coordinates.

$$\Sigma Q_i r_1^2 = \Sigma Q_i (x_i^2 + y_i^2 + z_i^2) = \text{Tr} \mathbf{q}$$
 3.10.4

If we have a single extended body in which the charge density ρ varies from point to point according to $\rho = \rho(x, y, z) \text{ Cm}^{-3}$, we can calculate the various moments in a similar way to that described in section 3.10 for masses.

Unlike in the case of point masses, there is little point in defining some point $(\bar{x}, \bar{y}, \bar{z})$ by some such equation as $Q\bar{x} = \sum Q_i x_i$ - particularly in such frequent cases in which the total charge is zero.

It is possible, however, (and sometimes useful) to find a point such that, when used as origin of coordinates, the trace (sum of the diagonal elements) is zero. Perhaps this is best seen with a numerical example. Let us suppose that we have a system of point charges as follows. However unrealistic it may be, I'll suppose that the charges are in coulombs and the coordinates in metres, in order to keep the numerical calculation simple in SI units.

Q_i	x_i	<i>Yi</i>	Z_i
8	4	-6	8
-12	2	-3	9
2	-8	7	10
2	5	4	-6

The total charge on the system is zero.

The dipole moment matrix is

$$\mathbf{q} = \begin{pmatrix} 258 & -192 & -180 \\ -192 & 310 & 32 \\ -180 & 32 & -188 \end{pmatrix} \qquad \qquad \mathbf{C} \ \mathbf{m}^2 \qquad \qquad 3.10.5$$

Now let us imagine moving the origin of the reference axes (without rotation), and as we do so the numbers in the matrix change. Sooner or later we may find that, when the origin of the axes reaches some point (a,b,c), the numbers in the matrix are such that

the trace (sum of the diagonal elements) is zero. This couldn't happen with a set of point masses, all of which have positive mass.

When the origin is at the point (a,b,c) the coordinates of the charges are.

Q_i	x_i	y_i	Z_i
8	4 <i>-a</i>	-6-b	8– <i>c</i>
-12	2-a	-3-b	9-с
2	-8-a	7 <i>-b</i>	10- <i>c</i>
2	5 <i>–a</i>	4 - <i>b</i>	-6-c

The diagonal elements of the quadrupole moment matrix are now

$$q_{xx} = 8 \times (4-a)^2 - 12 \times (2-a)^2 + 2 \times (-8-a)^2 + 2 \times (5-a)^2 = 258 - 4a$$

$$q_{yy} = 8 \times (-6-b)^2 - 12 \times (-3-b)^2 + 2 \times (7-b)^2 + 2 \times (4-b)^2 = 310 - 20b$$

$$q_{zz} = 8 \times (8-c)^2 - 12 \times (9-c)^2 + 2 \times (10-c)^2 + 2 \times (-6-c)^2 = -188 + 72c$$

The trace is $\text{Tr } \mathbf{q} = 380 - 4a - 20b + 72c$.

Thus, if we choose the origin of coordinates to be any point (a, b, c) that lies in the plane

$$x + 5y - 18z - 95 = 0, \qquad 3.10.6$$

the trace of the quadrupole moment matrix will be zero. That is, $\sum Qr_i^2 = 0$.

For example, we might choose the point $(0,0,\frac{95}{18})$ as our origin of coordinates. In that case the coordinates of the four point charges are

Q_i	x_i	y_i	Z_i
8	4	-6	$\frac{247}{18}$
-12	2	-3	$\frac{265}{18}$
2	-8	7	$\frac{283}{18}$
2	5	4	$-\frac{5}{18}$

and the quadrupole moment tensor in its matrix representation becomes

Its trace is zero.

Now, rather than bodily moving the origin from one place to another without rotation, let us keep the origin of coordinates fixed, but we'll rotate the system of coordinate axes (keeping them orthogonal, of course). As we do so, we'll see the elements of the matrix changing. However, regardless of whether we use the original origin (which gave us a nonzero trace) or the new origin (which gives us a zero trace), we'll notice that during the rotation the trace (sum of the diagonal elements) does not change. This is not in the least surprising, because the trace is ΣQr_i^2 and none of the r_i change as long as we keep the origin fixed. We may also find that there is one orientation of the axes which results in a matrix *whose off-diagonal elements are all zero*. You'd be lucky to stumble upon this special orientation by accident or by trial and error.

Some readers will know how to diagonalize a symmetric matrix by finding its eigenvalues and its eigenvectors. I gave a detailed example of how to do it in Section 2.18 of Chapter 2 in my notes on Classical Mechanics (<u>http://orca.phys.uvic.ca/~tatum/classmechs/class2.pdf</u>), so I'll just do it quickly here for the matrix given in equation 3.10.7. Some will want to skip this, and just see the answers.

First we have to find the eigenvalues of the matrix, which are given by the solution of the characteristic equation:

$$\begin{pmatrix} 258.0 - \lambda & -192.0 & -169.\dot{4} \\ -192.0 & 310.0 - \lambda & 84.\dot{7} \\ -169.\dot{4} & 84.\dot{7} & -568.0 - \lambda \end{pmatrix} = 0$$
 3.10.8

This is a cubic equation, and viewers who are new to this may find it straightforward but exceedingly tedious. However, once you have done it, and if you anticipate having to do this sort of thing often, you write a computer program for it so that in future you can do it instantly without having to remember all the details of how to do it. I dare say some programs, available online, such as Wolfram Alpha, can do it for you. In any case the three solutions of the above equation are

$$\lambda = 97.2 \quad 506.7 \quad -603.9$$

(More accurately they are 97.162854, 506.689881, -603.853736. In the text that follows, I have printed only a few significant figures; the actual calculations were done by computer in double precision.)

30

The quadrupole matrix when referred to the new axes is :

$$\mathbf{q} = \begin{pmatrix} 97.2 & 0 & 0 \\ 0 & 506.7 & 0 \\ 0 & 0 & -603.9 \end{pmatrix} \qquad \qquad \mathbf{C} \, \mathbf{m}^2 \qquad 3.10.9$$

This tells us what the diagonal elements are when referred to the new axes, but it doesn't tell us the orientation of the new axes. By the "orientation" I mean the direction cosines of the new axes when referred to the old axes. Let us call the direction cosines of

one of the new axes
$$\begin{pmatrix} l_1 \\ m_1 \\ n_1 \end{pmatrix}$$
. It must satisfy
 $\begin{pmatrix} 258.0 & -192.0 & -169.\dot{4} \\ -192.0 & 310.0 & 84.\dot{7} \\ -169.\dot{4} & 84.\dot{7} & -568.0 \end{pmatrix} \begin{pmatrix} l_1 \\ m_1 \\ n_1 \end{pmatrix} = 97.2 \begin{pmatrix} l_1 \\ m_1 \\ n_1 \end{pmatrix}$. 3.10.10

This looks like three linear equations in the three direction cosines l_1 , m_1 , n_1 . Unfortunately the three equations are not independent, the third being a linear combination of the other two. We need an additional equation, which is provided by the theorem of Pythagoras, which tells us that

$$l_1^2 + m_1^2 + n_1^2 = 1. 3.10.11$$

The first two equations implicit in 3.10.10 are

$$160.8\frac{l_1}{n_1} - 192\frac{m_1}{n_1} - 169.\dot{4} = 0 3.10.12$$

$$-192\frac{l_1}{n_1} + 212.8\frac{m_1}{n_1} + 84.\dot{7} = 0$$
 3.10.13

Combined with equation 3.10.11, these result in

$$l_1 = \pm 0.71984$$
 $m_1 = \pm 0.68750$ $n_1 = \pm 0.09575$ 3.10.14

You may choose either sign. The axis can go in either of these two opposite directions.

It should be verified, as a check, that these also satisfy the third equation implicit in 3.10.10, namely

$$-169.\dot{4}\frac{l_1}{n_1} + 84.\dot{7}\frac{m_1}{n_1} - 665.2 = 0 \qquad 3.10.15$$

(I have been working to double precision in the computer, but I have printed the numbers to only a few significant figures.)

In a similar manner you can find the direction cosines of the other two axes from

$$\begin{pmatrix} 258.0 & -192.0 & -169.\dot{4} \\ -192.0 & 310.0 & 84.\dot{7} \\ -169.\dot{4} & 84.\dot{7} & -568.0 \end{pmatrix} \begin{pmatrix} l_2 \\ m_2 \\ n_2 \end{pmatrix} = 506.7 \begin{pmatrix} l_2 \\ m_2 \\ n_2 \end{pmatrix}.$$
 3.10.16

and

$$\begin{pmatrix} 258.0 & -192.0 & -169.\dot{4} \\ -192.0 & 310.0 & 84.\dot{7} \\ -169.\dot{4} & 84.\dot{7} & -568.0 \end{pmatrix} \begin{pmatrix} l_3 \\ m_3 \\ n_3 \end{pmatrix} = -603.9 \begin{pmatrix} l_3 \\ m_3 \\ n_3 \end{pmatrix}.$$
 3.10.17

The results are:

$$l_2 = \pm 0.67006$$
 $m_2 = \pm 0.72424$ $n_2 = \pm 0.16278$ 3.10.18

$$l_3 = \pm 0.18126$$
 $m_3 = \pm 0.05302$ $n_3 = \pm 0.98201$ 3.10.19

While you are free to choose either sign for l_1 and l_2 , you are not quite free to do so for l_3 . The original axes were probably a right-handed system, and you probably want the new axes, after rotation, also to be right-handed.

First, you should check that

$$\begin{vmatrix} l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \\ l_3 & m_3 & n_3 \end{vmatrix} = \pm 1, \qquad 3.10.20$$

in which the vertical lines indicate the determinant of the matrix.

This checks that your three new axes are still orthogonal (at right angles to each other). If equation 3.10.20 is not satisfied, you have made an arithmetic mistake somewhere. In Section 2.18 of Chapter 2 in my notes on Classical Mechanics (<u>http://orca.phys.uvic.ca/~tatum/classmechs/class2.pdf</u>) I show how you can use the properties of an orthogonal matrix to locate very quickly where the mistake is. Then, if you want to make sure that you have not changed the chirality (handedness) of the axes, you choose the signs so that the matrix is +1, not -1. In our present case we find that

+0.71984	+0.68750	-0.09575	
+0.67006	-0.72424	-0.16278	= +1.
-0.18126	+0.05302	-0.98201	

If you wish to convert these direction cosines to Euler angles, refer to the above underlined blue link.

3.11 *Quadrupole Moment.* Potential near an arbitrary charge distribution.

We noted in Section 3.9 that there are so many "second moments of mass" that the mere unqualified term "moment of inertia" is open to some ambiguity, and not all writers may mean the same thing. We make a mental note always to make sure in our own writing that our readers will understand what we mean in a particular context. Likewise with distributions of electric charge, there are many "second moments of charge", and the mere unqualified term "quadrupole moment" is subject to similar ambiguity.

We are going to look in this section at the problem of calculating the electric potential in the vicinity of an arbitrary distribution of charge. It can be shown (we shall shortly do so) that the electric potential in the vicinity of an arbitrary distribution of charges can be written as a series of the form:

$$4\pi\varepsilon_0 V = \frac{c_0 P_0(\cos\theta)}{R} + \frac{c_1 P_1(\cos\theta)}{R^2} + \frac{c_2 P_2(\cos\theta)}{R^3} + \frac{c_3 P_3(\cos\theta)}{R^4} + \dots \qquad 3.11.1$$

Here the *P_i* are the Legendre polynomials. (obviously some knowledge if these will be needed in what follows. See, for example, Section 1.4 of http://orca.phys.uvic.ca/~tatum/celmechs/celm1.pdf)

The c_i are coefficients that are determined by the charge distribution and geometry of the system. They have dimensions as follows: $[c_0] = Q$ $[c_1] = QL$ $[c_2] = QL^2$ $[c_3] = QL^3$. We shall see shortly that c_0 is identified with the net *charge* Q of the system. Some writers will identify c_1 as "the" *dipole moment* of the system, and c_2 (or some simple multiple of it) as "the" *quadrupole* moment, and c_3 as "the" *octupole moment*. In this section we'll see what c_1 and c_2 really are.

Let us imagine that we have a charge Q_i at spherical coordinates (r_i, θ_i, ϕ_i) . See figure III.15. We shall aim to answer the question: What is the electrical potential *V* at a point P(R, θ, ϕ), expressed in terms of Q_i and the spherical coordinates of the charge and the point P?

The potential V at P is, of course, given by

$$4\pi\varepsilon_0 V = \frac{Q_i}{\Delta_i},\qquad 3.11.2$$

so the problem is just the geometrical one of expressing Δ_i in terms of (r_i, θ_i, ϕ_i) and (R, θ, ϕ) .

From the cosine rule of plane trigonometry we have

$$\Delta_i^2 = R^2 + r_i^2 - 2Rr_i \cos \omega_i, \qquad 3.11.3$$

and from the cosine rule of spherical trigonometry we have

$$\cos \omega_i = \cos \theta \cos \theta_1 + \sin \theta \sin \theta_1 \cos(\phi - \phi_i), \qquad 3.11.4$$

so we have now been able to express Δ_i in terms of the coordinates.

We can write equation 3.11.2 as

$$4\pi\varepsilon_0 V = \frac{Q_i}{R} \left[1 + \left(\frac{r_i}{R}\right)^2 - 2\left(\frac{r_i}{R}\right) \cos\omega_i \right]^{-1/2}$$
 3.11.5

We might if we wish choose our coordinate system so that the point P is on the *z*-axis, in which case ω_i is merely θ_i . In any case we can expand the expression in equation 3.11.5 as a series of Legendre polynomials. See equation 1.14.2 of www.astro.uvic.ca/~tatum/celmechs/celm1.pdf.

$$4\pi\varepsilon_0 V = \frac{Q_i}{R} \left[P_0(\cos\omega_i) + P_1(\cos\omega_i) \left(\frac{r_i}{R}\right) + P_2(\cos\omega_i) \left(\frac{r_i}{R}\right)^2 + P_3(\cos\omega_i) \left(\frac{r_i}{R}\right)^3 + \dots \right]^{-1/2}$$

$$3.11.6$$

If we have many point charges, not just one, the potential is calculated from

$$4\pi\varepsilon_0 V = \frac{1}{R} \sum_{i} Q_i \left[P_0(\cos\omega_i) + P_1(\cos\omega_i) \left(\frac{r_i}{R}\right) + P_2(\cos\omega_i) \left(\frac{r_i}{R}\right)^2 + P_3(\cos\omega_i) \left(\frac{r_i}{R}\right)^3 + \dots \right]^{-1/2}$$

$$3.11.7$$

Or if we have a single extended body, in which the the charge density (C m^{-3}) is a function of postion, it is calculated from

$$4\pi\varepsilon_0 V = \frac{1}{R} \int \rho \left[P_0(\cos\omega) d\tau + P_1(\cos\omega) \left(\frac{r}{R}\right) d\tau + P_2(\cos\omega) \left(\frac{r}{R}\right)^2 d\tau + P_3(\cos\omega) \left(\frac{r}{R}\right)^3 d\tau + \dots \right]^{-1/2}$$

3.11.8

Here $d\tau$ is the elemental volume dxdydz in cartesian coordinates, or $r^2 \sin \theta dr d\theta d\phi$ in spherical coordinates. The integration is to be carried out throughout the volume of the

body, or throughout all of space if it is assumed that the charge density is zero outside the body.

Now $P_0(\cos \omega) = 1$. Therefore the first term in equations 3.11.7 and 3.11.8 is merely $\frac{Q}{R}$, where Q is the total net charge of the system of point charges or of the extended body. The coefficient c_0 of equation 3.11.1 is identified with Q.

Further, $P_1(\cos \omega) = \cos \omega$. Reference to figure III.15 should convince the reader that $\sum_i Q_i r_i \cos \omega_i$, or $\int \rho r \cos \omega d\tau$, is the component of the dipole moment **p** of the system in the direction to P. I'll call this component p_0 . Thus the second term in equations 3.11.7 and 3.118 is $\frac{p_0}{R^2}$, and the coefficient c_1 of equation 3.11.1 is identified with p_0 .

We have, then, so far; $4\pi\epsilon_0 V = \frac{Q}{R} + \frac{P_0}{R^2}$ plus higher-order terms.

Finding the next term is a little more difficult, but it can be made much easier, with no loss of generalization, by referring everything to a set of coordinate axes such that the point P is on the *z*-axis. This will, of course mean, expressing the coordinates of each point charge to these axes, which may need some preliminary work.

With our now preferred axes, equations 3.11.7 and 3..11.8 become

$$4\pi\varepsilon_0 V = \frac{Q}{R} + \frac{P_z}{R^2} + \frac{1}{R^3} \sum_i Q_i r_i^2 P_2(\cos\theta_i) + \dots \qquad 3.11.9a$$

and

 $4\pi\varepsilon_0 V = \frac{Q}{R} + \frac{p_z}{R^2} + \frac{1}{R^3} \int \rho r^2 P_2(\cos\theta) d\tau + \dots \qquad 3.11.9b$

(Referred to these axes, what we called p_0 is now p_z)

Now $P_2(\cos \theta) = \frac{1}{2}(3\cos^2 \theta - 1)$. Therefore the third term is equation 3.11.9a is

$$\frac{1}{2} \left(3\sum_{i} Q_{i} r_{i}^{2} \cos^{2} \theta_{i} - \Sigma Q_{i} r_{i}^{2} \right) = \frac{1}{2R^{3}} \left(3\sum_{i} Q_{i} z_{i}^{2} - \Sigma Q_{i} r_{i}^{2} \right)$$
$$= \frac{1}{2R^{3}} (3q_{zz} - \operatorname{Tr} \mathbf{q}) = \frac{1}{2R^{3}} (2q_{zz} - q_{xx} - q_{yy}).$$

3.11.10

Here **q** is the diagonalized quadrupole moment matrix. Thus the potential (whether of a system of charges or a single extended body) at a point P situated on the *z*-axis at a distance *R* from the origin is given by

$$4\pi\varepsilon_0 V = \frac{Q}{R} + \frac{p_z}{R^2} + \frac{1}{2R^3}(2q_{zz} - q_{xx} - q_{yy}) + \dots \qquad 3.11.11$$

The coefficient c_2 of equation 3.11.1 is now identified as $\frac{1}{2}(2q_{zz} - q_{xx} - q_{yy})$. I believe the quantity $2q_{zz} - q_{xx} - q_{yy}$ is referred to by some writers as "the" quadrupole moment, though it is hard to tell if an author does not explicitly refine his or her terms."

3.12 Two simple quadrupoles

Neither of the two systems shown in figure III.16 has a net charge or a net dipole moment, and neither will experience a force or a torque in a uniform field. Both of them have quadropole (and higher-order) moments, and both may (depending on the geometry of the field) experience a force or a torque is a nonuniform field.

Let us look at system (a), and we'll start by putting the system along the z-axis of the cartesian coordinate system, with the -2Q charge at the origin. There will be no loss of

generality if we put the point P in he *zx*-plane. The cartesian coordinates of P are (x,0,z) and its spherical coordinates are $(r, \theta, 0)$. See figure III.17.

FIGURE III.17

The potential at P is given (exactly) by:

$$4\pi\varepsilon_{0}V = \frac{Q}{\Delta_{1}} - \frac{2Q}{r} + \frac{Q}{\Delta_{2}} = \frac{Q}{r\sqrt{1 - 2(\frac{a}{r})\cos\theta + (\frac{a}{r})^{2}}} - \frac{2Q}{r} + \frac{Q}{r\sqrt{1 + 2(\frac{a}{r})\cos\theta + (\frac{a}{r})^{2}}}.$$
(3.12.1)

That expression is exact for the potential at a point (r, θ) and straightforward to calculate - so why would one ever want to find an approximate expression? Well, suppose we wanted to draw the equipotentials (and the lines of force, which are orthogonal to the equipotentials). We would want to re-cast equation 3.12.1 in the form $r = r(\theta; V)$. If you try this, you will see the difficulty. One could probably write it as $\cos \theta$ as a function of r and V, which would enable you to draw the exact equipotentials, but unless you want to do this very close to the linear quadrupole, an approximation may well suffice.

To obtain an approximation for the potential at a large distance, expand this as far as $\left(\frac{a}{r}\right)^2$ (or further if you wish). Then V is given approximately by

$$4\pi\varepsilon_{0}V = \frac{Q}{r} \Big[(P_{0}(\cos\theta) + P_{1}(\cos\theta)(\frac{a}{r}) + P_{2}(\cos\theta)(\frac{a}{r})^{2} + \dots - 2 + P_{0}(\cos\theta) - P_{1}(\cos\theta)(\frac{a}{r}) + P_{2}(\cos\theta)(\frac{a}{r})^{2} - \dots \Big]$$

$$= \frac{2Q}{r} \Big[P_{0}(\cos\theta) + P_{2}(\cos\theta)(\frac{a}{r})^{2} - 1 \Big]$$

$$3.12.2$$

Make use of $P_0(x) = 1$, $P_2(x) = \frac{1}{2}(3x^2 - 1)$, and this becomes just

$$4\pi\epsilon_0 V = \frac{Q}{r} (3\cos^2\theta - 1).$$
 3.12.3

At a large distance from the quadrupole, the equation to the equipotentials is

$$r = \frac{Q}{4\pi\epsilon_0 V} (3\cos^2\theta - 1) = \frac{\frac{1}{2}Q}{4\pi\epsilon_0 V} (3\cos 2\theta + 1)$$
 3.12.4

This is shown in figure III.18 for V = 0.25, 0.50, 1.00, 2.00 and 4.00 times $\frac{Q}{4\pi\varepsilon_0}$.

To find the equation to the lines of force we differentiate calculate $\frac{1}{r}\frac{dr}{d\theta}$

$$\frac{1}{r}\frac{dr}{d\theta} = -\frac{6\sin 2\theta}{3\cos 2\theta + 1}$$
3.12.5

Then replacement of $\frac{1}{r} \frac{dr}{d\theta}$ with $-r \frac{d\theta}{dr}$ will give the differential equation to the

orthogonal trajectories - i.e. to the lines of force:

$$r\frac{d\theta}{dr} = \frac{6\sin 2\theta}{3\cos 2\theta + 1}$$
 3.12.6

The integral of this equation, i.e. the equation to the lines of force, is

$$r = a[\sin^2 2\theta(1 - \cos 2\theta)]^{1/12}$$
 3.12.7

In figure III.19 we see, in black, the equipotentials for V = 0.25, 0.50, 1.00, 2.00 and 4.00

times
$$\frac{Q}{4\pi\varepsilon_0}$$
 and, in red, the lines of force for $\frac{r}{a} = 1, 2, 4, 8$.

FIGURE III.18

Readers will understand that these curves are approximations for large r/a. To draw the exact equipotentials close to the dipole, we need equation 3.12.1. It may not be easy to write this equation expressing r explicitly in terms of θ and V. It may be less difficult to write it expressing $\cos \theta$ in terms of r and V. If you can do this you should be able to plot the equipotentials. If any reader manages to do this, I would be happy to incorporate the result, with acknowledgment, of course, in these notes. You can find me at jtatum at uvic dot ca

It should be possible to repeat the analysis for the system (b) of figure III.16. There will be four distances to be expressed in terms of r and θ . These can be expanded in Legendre polynomials. When all four are added, the first two terms should be zero, and the third term will be the required equation to the equipotentials. Again, if anyone succeeds in doing this, let me know and we can incorporate it in these notes.

3.13 Octupole Moments

Look at the three-dimensional system of figure III.20.

FIGURE III.20

It has no net charge, no dipole moment, and no quadrupole moment. It does, however have an octupole moment, and higher-order moments. I suppose one might use the symbol $\mathbf{0}$ for octupole moment. It would be a tensor of the third rank, and its matrix representation would be a three-dimensional matrix, which would require three sheets of paper piled one upon another. Its 27 elements (not all of which are distinct) would each have three subscripts, of the kinds xxx, xyz, zzx, etc. One could find the potential at a point by the methods of the previous section - it would just be a bit more tedious. I'm not going to pursue that further here. As Sir Isaac Newton said, of a quite different but even more difficult problem: It doth make my head ake.

Just one remark. Figure III.20 might look as though it represents a unit cell of a sodium chloride crystal. It does to some extent, but you must bear in mind that the radii of the electron clouds of the sodium and the chloride ions are comparable in size to the size of the cube. The outermost electrons in effect fill up most of the cube. However, to the extent that the potential at a point external to a spherically-symmetry charge distribution is the same as if all the charge were concentrated at a point, figure III.20 might, for the purpose of calculating the potential at some distance from the cube, be a reasonable representation of sodium chloride.