The Multipole Expansion

Oct 25

In the previous lecture, we saw that the most general solution of Laplace's equation which tends to 0 as $r \to \infty$ has the form

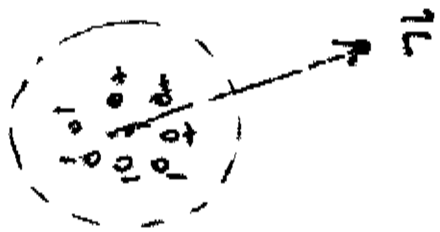
$$\varphi = \sum_{lm} \frac{B_{lm}}{r^{l+1}} Y_{lm}(\theta,\phi)$$

and

$$\varphi = \sum_{l} \frac{B_l}{r^{l+1}} P_l(\cos\theta) \qquad B_l = \left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}}$$

in the cylindrically symmetric case. So, some charge distributions lead to a $\varphi \sim \frac{1}{r}$, others to a $\varphi \sim \frac{1}{r^2}$, others to $\varphi \sim \frac{1}{r^3}$, etc. What, physically, leads to the difference?

To study this systematically, analyze as follows: Let $\rho(\vec{x})$ be a distribution of charge localized inside a sphere of radius R. Let $\vec{r}$ be a point outside the sphere: $|\vec{r}| > R$



Then the electrostatic potential at $\vec{r}$ is given by

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int d^3x \quad \rho(\vec{x}) \, \frac{1}{|\vec{r}-\vec{x}|}$$

Our setup implies that $|\vec{x}| < R < |\vec{r}|$, so if we Taylor expand the factor $|\vec{r}-\vec{x}|^{-1}$ in the components of $\vec{x}$, the Taylor series will converge. Let's see what happens when we do this:

$$|\vec{r}-\vec{x}|^{-1} = [r^2 - 2\vec{r}\cdot\vec{x} + x^2]^{-1/2}$$

$$= \frac{1}{r}\left[1 - 2\frac{\vec{r}\cdot\vec{x}}{r^2} + \frac{x^2}{r^2}\right]^{-1/2}$$

$$= \frac{1}{r}\Big[1 - \tfrac{1}{2}\left(-2\frac{\vec{r}\cdot\vec{x}}{r^2} + \frac{x^2}{r^2}\right)$$

$$+ \left(\frac{(-\frac{1}{2})(-\frac{3}{2})}{2!}\right)\left(-2\frac{\vec{r}\cdot\vec{x}}{r^2} + \frac{x^2}{r^2}\right)^2$$

$$+ \frac{(-\frac{1}{2})(-\frac{3}{2})(-\frac{5}{2})}{3!}\left(-2\frac{\vec{r}\cdot\vec{x}}{r^2} + \frac{x^2}{r^2}\right)^3$$

$$+ \cdots \Big]$$

The leading term is $\frac{1}{r}$, and you can see that the succeeding terms decrease as higher and higher powers of $\frac{1}{r}$.

Let's collect terms for the first few powers of $\frac{1}{r}$. For clarity, write $\frac{\vec{r}\cdot\vec{x}}{r^2} = \frac{\hat{r}\cdot\vec{x}}{r}$. Then

$$
\begin{aligned}
|\vec{r}-\vec{x}|^{-1} = \frac{1}{r}\Big[\, 1 &+ \frac{\hat{r}\cdot\vec{x}}{r} - \frac{1}{2}\frac{x^2}{r^2} \\
&+ \frac{3}{2}\frac{(\hat{r}\cdot\vec{x})^2}{r^2} - \frac{3}{2}\frac{\hat{r}\cdot\vec{x}\, x^2}{r^3} + \frac{3}{8}\frac{x^4}{r^4} \\
&+ \frac{5}{2}\frac{(\hat{r}\cdot\vec{x})^3}{r^3} - \frac{15}{4}\frac{(\hat{r}\cdot\vec{x})^2 x^2}{r^4} \\
&+ \frac{35}{8}\frac{(\hat{r}\cdot\vec{x})^4}{r^4} \\
&+ \cdots \Big]
\end{aligned}
$$

so

$$
\begin{aligned}
\varphi(r) &= \frac{1}{4\pi\epsilon_0}\int d^3x\, \rho(\vec{x}) \cdot \\
&\cdot \Big\{ \frac{1}{r} + \frac{\hat{r}\cdot\vec{x}}{r^2} + \frac{1}{r^3}\left(\frac{3}{2}(\hat{r}\cdot\vec{x})^2 - \frac{1}{2}x^2\right) \\
&+ \frac{1}{r^4}\left(\frac{5}{2}(\hat{r}\cdot\vec{x})^3 - \frac{3}{2}(\hat{r}\cdot\vec{x})x^2\right) \\
&+ \frac{1}{r^5}\left(\frac{35}{8}(\hat{r}\cdot\vec{x})^4 - \frac{15}{4}(\hat{r}\cdot\vec{x})^2x^2 + \frac{3}{8}x^4\right) \\
&+ \mathcal{O}\left(\frac{1}{r^6}\right) \Big\}
\end{aligned}
$$

If we set $\hat{r}\cdot\hat{x} = \cos\theta_{rx}$ we can recognize Legendre polynomials:

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0}\int d^3x\ \rho(\vec{x})\left\{\frac{1}{r} + \frac{x}{r^2}P_1(\cos\theta_{rx}) + \frac{x^2}{r^3}P_2(\cos\theta_{rx}) + \cdots\right\}$$

This is not a surprise, since

$$\frac{1}{|\vec{r}-\vec{x}|} = \frac{1}{\left[r^2 - 2\vec{r}\cdot\vec{x} + x^2\right]^{\frac{1}{2}}} = \frac{1}{r}\,\frac{1}{\left[1 - 2\frac{x}{r}\cos\theta_{rx} + x^2/r^2\right]^{\frac{1}{2}}}$$

$$= \frac{1}{r}\,T\left(\cos\theta_{rx}, \frac{x}{r}\right)$$

where T is the generating function of Legendre polynomials. We will see Legendre polynomials appearing in another context later in this analysis.

The first term in our expansion for $\varphi(\vec{r})$ is:

$$\varphi(r) = \frac{1}{4\pi\epsilon_0}\left[\int d^3x\ \rho(\vec{x})\right]\frac{1}{r} + O\left(\frac{1}{r^2}\right)$$

We recognize the coefficient as the total charge of the configuration

$$Q = \int d^3x\ \rho(\vec{r})$$

So we see ~~that~~ the potential of a localized charge distribution behaves as $\frac{1}{r}$ as $r \to \infty$ precisely when the total charge is nonzero.

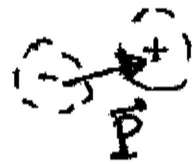
If the total charge is zero, the leading term in φ

is :

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0} \left[\int d^3x\, \rho(\vec{x})\, \vec{x}\right] \cdot \frac{\hat{r}}{r^2}$$

The coefficient is a vector associated with the charge distribution, which points from regions of excess negative charge to regions of excess positive charge!

$$\vec{P} = \left[\int d^3x\, \rho(\vec{x})\, \vec{x}\,\right]$$



When $Q = 0$ but $\vec{P} \neq 0$, φ falls off as $1/r^2$. $\vec{P}$ is called the polarization or dipole moment.

Similarly, we can write the higher terms in the series for φ in terms of integrals over the charge distribution:

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0} \left(\frac{Q}{r} + \frac{\vec{P}\cdot\hat{r}}{r^2} + \frac{1}{2r^3}\, \hat{r}_i\, Q_{ij}\, \hat{r}_j \right.$$

$$\left. + \frac{1}{2r^4}\, \hat{r}_i \hat{r}_j \hat{r}_k\, Q^{(3)}_{ijk} + \cdots \right)$$

where

$Q = \int d^3x\, \rho(\vec{x})$ "monopole moment" = charge

$\vec{P} = \int d^3x\, \rho(\vec{x})\, \vec{x}$ "dipole moment" = polarization

$Q_{ij} = \int d^3x\, \rho(\vec{x}) \left[3x^i x^j - \delta^{ij} x^2\right]$ "quadrupole moment"

This expansion is called the "multipole expansion", and the successive terms are called the monopole, dipole, quadrupole, octupole, etc terms. It is amazing that, up to any given power of $1/r$, the electrostatic potential is independent of the detailed form of the charge distribution but depends only on the values of the "multipole moments" — integrals over the charge distribution — up to that order.

You are very familiar with the monopole electric field, the field of a $\frac{1}{r}$ potential. It would be good to become familiar also with the fields of a pure dipole and a pure quadrupole

For a dipole,

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{\vec{P}\cdot\hat{r}}{r^2} = \frac{1}{4\pi\epsilon_0}\frac{P^j r^j}{r^3}$$

$$E^i = -\left(\frac{\partial}{\partial x^i}\right)\varphi = \frac{1}{4\pi\epsilon_0}\left(\frac{3}{r^5} r^i \cdot P^j r^j - \frac{1}{r^3} P^i\right)$$

$$= \frac{1}{4\pi\epsilon_0}\frac{[3r^i r^j - \delta^{ij} r^2]}{r^5} P^j$$

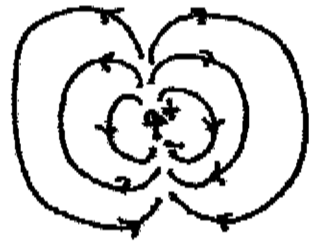
for a dipole that points in the $\hat{z}$ direction

$$\vec{P} = P\hat{z}$$

$$E^i = \frac{1}{4\pi\epsilon_0} \frac{3 r^i r \cos\theta - \delta^{iz} r^2}{r^5} P$$

so that

$$E^x = \frac{1}{4\pi\epsilon_0} \frac{3\cos\theta\sin\theta\cos\phi}{r^3}$$



$$E^y = \frac{1}{4\pi\epsilon_0} \frac{3\cos\theta\sin\theta\sin\phi}{r^3}$$

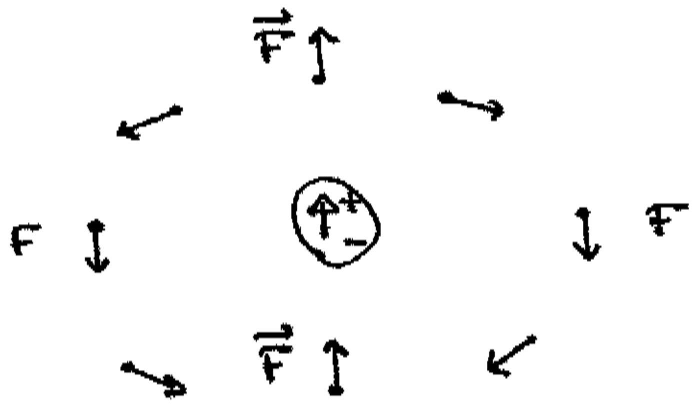
$$E^z = \frac{1}{4\pi\epsilon_0} \frac{3\cos^2\theta - 1}{r^3}$$

This E field falls off like $\frac{1}{r^3}$; its direction depends strongly on the position $\vec{r}$ and the orientation of the dipole.

For a charge Q' in the field of the dipole

$$\vec{F} = \frac{Q'}{4\pi\epsilon_0} \frac{3\hat{r}\ \hat{r}\cdot\vec{P} - \vec{P}}{r^3}$$

<u>$Q' > 0$</u>



Now what if we put in the field of the dipole a body with zero total charge but which is polarized and so has a dipole moment of its own.

It would be good to work out a more general formalism to treat this situation. Consider two charge distributions, one localized near $\vec{r}=0$, the other localized near $\vec{r}=\vec{r}_0$

$$\vec{y} = \vec{r} - \vec{r}_0$$

If these charge distributions are well separated compared to their sizes, the charges in ρ' feel the multipole potential set up by ρ.

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0}\left(\frac{Q}{r} + \frac{\vec{P}\cdot\hat{r}}{r^2} + \cdots\right)$$

The potential energy of the charges in the distribution ρ' is

$$V = \int d^3\vec{r}\ \rho'(\vec{r})\,\varphi(\vec{r})$$

$$= \int d^3\vec{y}\ \rho'(\vec{y})\,\varphi(\vec{r}_0+\vec{y})$$

since $|\vec{y}| \ll |\vec{r}_0|$, it makes sense to Taylor expand the potential

$$V = \int d^3y \; \rho'(\vec{y}) \left[\varphi(\vec{r}_0) + \vec{y} \cdot \frac{\partial}{\partial \vec{r}_0} \varphi + \frac{1}{2} y^i y^j \frac{\partial^2}{\partial r_0^i \partial r_0^j} \varphi + \cdots \right]$$

For a monopole field $\varphi \sim \frac{1}{r_0}$ $\frac{\partial}{\partial r_0^i} \varphi \sim \frac{1}{r_0^2}$ $\cdots$

For a dipole field $\varphi \sim \frac{1}{r_0^2}$ $\frac{\partial}{\partial r_0^i} \varphi \sim \frac{1}{r_0^3}$ $\cdots$

In any case if $|\vec{y}| \ll |\vec{r}_0|$, the leading nonzero term will dominate the potential energy.

If the distribution ρ' has a monopole moment

$$\int d^3y \; \rho'(y) = Q' \neq 0$$

this term dominates and we obtain

$$V \cong Q' \varphi(r_0) + \cdots$$

where the terms omitted are smaller by $\frac{Y}{r_0}$, where Y is the size of the charge distribution. That is, the charge distribution behaves approximately like a charge Q' with no other structure.

If the monopole moment vanishes

$$Q' = 0$$

we can look at the next term, which is proportional to the dipole moment

$$\vec{P}' = \int d^3y \; \rho'(\vec{y}) \; \vec{y}$$

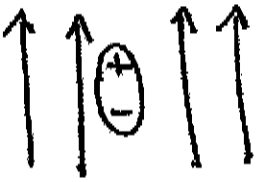
this term is

$$V \cong \vec{P}' \cdot \vec{\nabla}\varphi(\vec{r}_0) + \cdots$$

or

$$V = -\vec{P}' \cdot \vec{E}(\vec{r}_0) + \cdots$$

again, the error is of relative size $\frac{r}{r_0}$. According to this formula, a point dipole likes to be aligned with an electric field



has lower energy than

A dipole misaligned with an electric field can also lower its energy by moving to where the field is smaller.

Putting in the explicit formula for the electric field of a dipole, we can compute the potential energy of interaction of two dipoles:

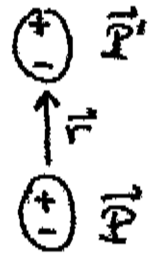
$$V = -P'^{i} \frac{1}{4\pi\epsilon_0} \frac{3r^i r^j - \delta^{ij} r^2}{r^5} P^j$$

or

$$V = -\frac{1}{4\pi\epsilon_0}\left(\frac{3\hat{r}\cdot\vec{P}\;\hat{r}\cdot\vec{P}' - \vec{P}\cdot\vec{P}'}{r^3}\right)$$

This potential energy goes as $1/r^3$, so the force between dipoles is $1/r^4$. But nothing else about this formula is simple. The potential energy depends on the relative alignment of $\vec{P}$ and $\vec{P}'$ and on their orientation with respect to $\hat{r}$. For example:

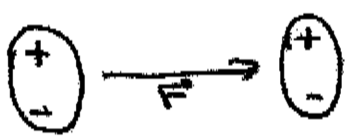
$\vec{P}, \vec{P}', \hat{r}$ all parallel:



$$V = -\frac{2}{4\pi\epsilon_0}\frac{PP'}{r^3}$$

attractive

$\vec{P}\,\vec{P}'$ parallel, $\perp$ to $\hat{r}$



$$V = +\frac{1}{4\pi\epsilon_0}\frac{PP'}{r^3}$$

repulsive

The average of V over relative orientations can be compute from

$$\langle r^i r^j \rangle = \frac{1}{3} r^2 \delta^{ij}$$

[the average over orientations must be $\propto \delta^{ij}$; to check the coefficient, set $i=j$ and sum.] Then

$$\langle V \rangle = -\frac{1}{4\pi\epsilon_0}\left\langle\frac{(3\hat{r}^i\hat{r}^j - \delta^{ij})}{r^3}\right\rangle P^i P'^j$$

$$= -\frac{1}{4\pi\epsilon_0}\frac{(3\cdot\frac{1}{3}\delta^{ij} - \delta^{ij})}{r^3} P^i P'^j \quad = 0 \;!$$

Let's go back and consider one more term in the series on p.5. If $Q=0$ and $\vec{P}=0$, the leading term in φ is

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0}\frac{1}{2r^3} Q_{ij}\,\hat{r}_i\hat{r}_j$$

where the quadrupole moment Q_{ij} is given by

$$Q_{ij} = \int d^3x\,\rho(\vec{x})\,(3x^i x^j - \delta^{ij}x^2)$$

Q_{ij} is a 3x3 matrix of moments of the charge distribution. Notice that it is a symmetric matrix: $Q_{ij} = Q_{ji}$

Q_{ij} also has the property that it is traceless:

$$\text{trace}\,Q = \sum_i Q_{ii} \;;$$

$$Q \text{ is traceless if } \sum_i Q_{ii} = 0.$$

If you think of Q_{ij} as carrying two vector indices, this condition is a dot product and so is rotationally invariant; if Q_{ij} is traceless in one coordinate system, it is traceless in any coordinate system. Now check:

$$Q_{ii} = \int d^3x\,\rho(x)\,(3x^i x^i - \delta^{ii}x^2)$$

$$= \int d^3x\,\rho(x)\,(3x^2 - 3x^2) = 0$$

The fact that Q_{ij} is traceless tells us that Q_{ij} has to do with the distribution of charge among the three axes and vanishes if the charge distribution is isotropic. To picture this, think about the case in which the distribution $\rho(x)$ is cylindrically symmetric. Then

$$\int d^3x\, \rho(x)\, (x^1)^2 = \int d^3x\, \rho(x)\, (x^2)^2$$

$$\int d^3x\, \rho(x)\, x^1 x^2 = \int d^3x\, \rho(x)\, x^1 x^3 = \int d^3x\, \rho(x)\, x^2 x^3 = 0$$

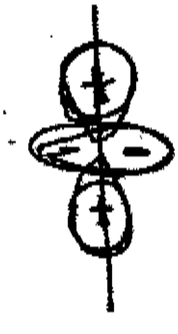
then

$$Q_{11} = \int d^3x\, \rho(x)\, (3(x^1)^2 - x^2) = Q_{22}$$

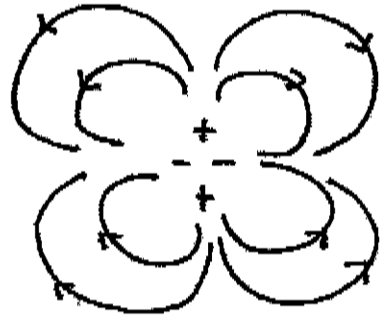
$$Q_{33} = \int d^3x\, \rho(x)\, (3(x^3)^2 - x^2)$$

and $\quad Q_{11} + Q_{22} + Q_{33} = 0$

If $Q_{33} > 0 \qquad Q_{11}, Q_{22} < 0$, the charge distribution has the form:



and you can imagine — or calculate — the corresponding set of E fields:



It is instructive to work out $\varphi(\vec{r})$ in this case; since

$$Q_{11} = Q_{22} = -\frac{1}{2} Q_{33}$$

$$\varphi(\vec{r}) = \frac{1}{4\pi\epsilon_0} \frac{1}{2r^3} Q_{33}\left((\hat{r}^3)^2 - \frac{1}{2}[(\hat{r}^1)^2 + (\hat{r}^2)^2]\right)$$

since $(\hat{r}^1)^2 + (\hat{r}^2)^2 + (\hat{r}^3)^2 = 1$ $\hat{r}$ is a unit vector

$$= \frac{1}{4\pi\epsilon_0} \frac{1}{2r^3} Q_{33}\left((\hat{r}^3)^2 - \frac{1}{2}[1-(\hat{r}^3)^2]\right)$$

$$= \frac{1}{4\pi\epsilon_0} \frac{1}{2r^3} Q_{33}\left(\frac{3}{2}(\hat{r}^3)^2 - \frac{1}{2}\right)$$

Finally $\hat{r}^3 = \cos\theta$ so.

$$\varphi(\vec{r}) = \frac{Q_{33}}{8\pi\epsilon_0 r^3}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right) = \frac{Q_{33}}{8\pi\epsilon_0 r^3} P_2(\cos\theta)$$

It is also true for the higher multipoles that the assumption of cylindrical symmetry of ρ brings these into the form

$$\varphi \sim (\text{const}) \cdot \frac{1}{r^{l+1}} P_l(\cos\Theta)$$

as required from the analysis of the previous lecture.

What about more general charge distributions? Since Q_{ij} is a symmetric matrix, it leads to a self-adjoint eigenvalue problem. Thus, Q_{ij} always has three mutually orthogonal eigenvectors v_a:

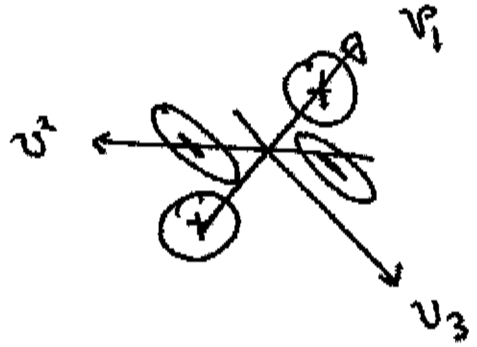
$$Q_{ij} (v_a)_j = \mathcal{Q}_a (v_a)_j \qquad a = 1, 2, 3$$

These vectors are called the principal axes of the charge distribution. The eigenvalues $\mathcal{Q}_a$ satisfy

$$\mathcal{Q}_1 + \mathcal{Q}_2 + \mathcal{Q}_3 = 0$$

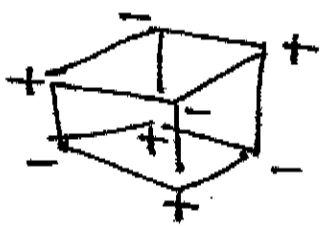
since Q_{ij} must be traceless in the coordinate system of the $\vec{v}_a$. If $\mathcal{Q}_1 > 0$, $\mathcal{Q}_2, \mathcal{Q}_3 < 0$, the positive charge extends along $\vec{v}_1$, and the negative charge extends outward in the plane of $\vec{v}_2$ $\vec{v}_3$:

for example,



If Q, $\vec{P}$, and Q_{ij} all vanish, the next possibility is an octopole, a charge distribution that is polarized internally, but not along any special axis,

for example

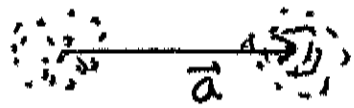


An arbitrary charge distribution can be represented as a sum of higher and higher multipoles. But, there is a technical comment that should be made. Let $\rho(\vec{x})$ be a distribution with $Q \neq 0$.

$$Q = \int d^3x \, \rho(\vec{x}) \qquad \vec{P} = \int d^3x \, \rho(\vec{x}) \, \vec{x} \quad \cdots$$

Now move this distribution by an amount $\vec{a}$. The new charge distribution is $\rho'(\vec{x}) = \rho(\vec{x}-\vec{a})$.

The (−) sign takes thinking about, but it is right; if the peak of the old distribution occurred at $\vec{x}=0$,



the peak of the new distribution is at $\vec{x}-\vec{a}=0$, i.e. at $\vec{x}=\vec{a}$.

Let's compute the multipole moments of the new distribution: $(\vec{x}' = \vec{x}-\vec{a})$

$$Q' = \int d^3x\, \rho(\vec{x}-\vec{a}) = \int d^3x'\, \rho(\vec{x}') = Q$$

$$\vec{P}' = \int d^3x\, \rho(\vec{x}-\vec{a})\, \vec{x} = \int d^3x'\, \rho(\vec{x}')(\vec{x}'+\vec{a}) = \vec{P} + Q\vec{a}$$

$$Q'_{ij} = \int d^3x\, \rho(\vec{x}-\vec{a})(3x^i x^j - \delta^{ij} x^2)$$

$$= \int d^3x'\, \rho(x')\left[3(x'+a)^i (x'+a)^j - \delta^{ij}(x'+a)^2\right]$$

$$= \int d^3x'\, \rho(x')\Big[(3x'^i x'^j - \delta^{ij} x'^2) + 3(x'^i a^j + x'^j a^i) - \delta^{ij}\, 2\vec{x}'\cdot\vec{a} + 3a^i a^j - \delta^{ij} a^2\Big]$$

$$= Q_{ij} + 3(P^i a^j + P^j a^i) - \delta^{ij}\, \vec{P}\cdot\vec{a} + (3a^i a^j - \delta^{ij} a^2)\, Q$$

Notice that if $Q = 0$, $\vec{P}$ is independent of $\vec{a}$ and reflects only the intrinsic form of the charge distribution. However, if $Q \neq 0$, $\vec{P}$ depends on the location of the charge distribution. A similar conclusion applies to Q_{ij}. In general,

if Q, $\vec{P}$, Q_{ij} ... is the first nonvanishing multipole moment, it depends only on the intrinsic properties of the charge distribution and not on the location of the charge distribution. All higher moments do depend on the location.