24 October 95

Multipoles and Energy

Consider a localized charge distribution $\rho(\vec{r})$ in an external potential $\Phi(\vec{r})$. [No part of $\Phi(\vec{r})$ is due to $\rho(\vec{r})$.] The interaction potential energy is:

$$U = \int d^3\vec{r}\ \rho(\vec{r})\Phi(\vec{r})$$

This will not contain any infinite self-energies.

Expand the potential in a Taylor Series:

$$\Phi(\vec{r}) = \Phi(0) + \vec{r}\cdot\vec{\nabla}\Phi(\vec{r})\Big|_{\vec{r}=0} + \frac{1}{2}\sum_i\sum_j x_i x_j \frac{\partial^2}{\partial x_i\,\partial x_j}\Phi(\vec{r})\Big|_{\vec{r}=0} + \cdots$$

In the linear term write: $\vec{\nabla}\Phi(\vec{r})\Big|_{\vec{r}=0} = -\vec{E}(0)$

Add to the quadratic term: $-\frac{1}{6}r^2\vec{\nabla}\cdot\vec{E}(\vec{r})\Big|_{\vec{r}=0} = 0$

since $\vec{\nabla}\cdot\vec{E} = 0$, this changes nothing.

$$\Phi(\vec{r}) = \Phi(0) - \vec{r}\cdot\vec{E}(0) - \frac{1}{6}\sum_i\sum_j\left(3x_i x_j - r^2\delta_{ij}\right)\frac{\partial E_j(\vec{r})}{\partial x_i}\Big|_{\vec{r}=0} + \cdots$$

$$U = q\Phi(0) - \vec{\mu}\cdot\vec{E}(0) - \frac{1}{6}\sum_i\sum_j Q_{ij}\frac{\partial E_j(\vec{r})}{\partial x_i}\Big|_{\vec{r}=0} + \cdots$$

Notice how the different multipole moments of $\rho(\vec{r})$ combine in the energy with $\Phi(\vec{r})$. We illustrate with the interaction potential energy of two dipoles.

To use the formalism we just developed, we must relegate one dipole ($\vec{\mu}_1$) to $\rho(\vec{r})$ and the other ($\vec{\mu}_2$) to $\Phi(\vec{r})$.

If $\vec{\mu}_2$ is at the origin then

$$\Phi(\vec{r}) = \frac{\vec{\mu}_2 \cdot \vec{r}}{r^3}$$

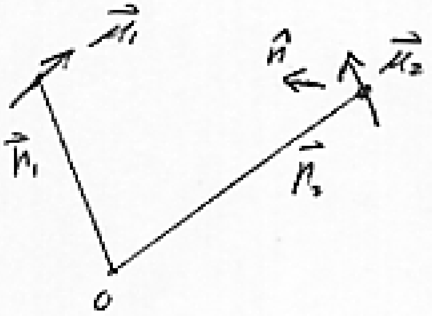
If $\vec{\mu}_2$ is at $\vec{r}\,'$ then

$$\Phi(\vec{r}) = \frac{\vec{\mu}_2 \cdot (\vec{r} - \vec{r}\,')}{|\vec{r} - \vec{r}\,'|^3}$$

The first dipole $\vec{\mu}_1$ will combine with the electric field due to the second in the energy U.

$$\vec{E}(\vec{r}) = -\vec{\nabla}\Phi(\vec{r}) = \frac{3\hat{n}(\vec{\mu}_2 \cdot \hat{n}) - \vec{\mu}_2}{|\vec{r} - \vec{r}\,'|^3} \qquad \text{where } \hat{n} = \frac{\vec{r} - \vec{r}\,'}{|\vec{r} - \vec{r}\,'|}$$

$$U_{12} = U_{21} = \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\hat{n} \cdot \vec{\mu}_1)(\hat{n} \cdot \vec{\mu}_2)}{|\vec{r}_1 - \vec{r}_2|^3} \qquad \text{where } \hat{n} = \frac{\vec{r}_1 - \vec{r}_2}{|\vec{r}_1 - \vec{r}_2|}$$



$U_{12} > 0$ is repulsion

$U_{12} < 0$ is attraction