Interaction Energy Between Two Disjoint Charge Distributions

We now have the machinery to calculate the interaction energy between two disjoint charge distributions. Suppose these distributions are clustered around the points $\vec{R}_a$ and $\vec{R}_b$ and suppose that the multipole moments of both distributions, relative to $\vec{R}_a$ & $\vec{R}_b$ are $Q^a, \mu^a_\alpha, \Theta^a_{\alpha\beta}, \Omega^a_{\alpha\beta\gamma}, \cdots$ and $Q^b, \mu^b_\alpha, \Theta^b_{\alpha\beta}, \Omega^b_{\alpha\beta\gamma}, \cdots$. The energy of distribution *b*, in the potential generated by distribution *a* is

$$V_{ab} = Q^b \phi^a(\vec{R}_{ab}) - \mu^b_\alpha F^a_\alpha(\vec{R}_{ab}) - \frac{1}{3}\Theta^b_{\alpha\beta} F^a_{\alpha\beta}(\vec{R}_{ab}) - \frac{1}{15}\Omega^b_{\alpha\beta\gamma} F^a_{\alpha\beta\gamma}(\vec{R}_{ab}) -$$

where $\vec{R}_{ba} = \vec{R}_b - \vec{R}_a$. For notational simplicity and with no loss of generality we will take $\vec{R}_a = 0$ and drop the subscript on $\vec{R}_b$. So distribution *a* is clustered about the origin and distribution *b* about the point $\vec{R}$. The energy due to the charge on *b* is then

$$Q^b \phi^a(\vec{R}) = \frac{Q^b Q^a}{R} - Q^b T^a_\alpha \mu^a_\alpha + \frac{1}{3} Q^b T^a_{\alpha\beta} \Theta^a_{\alpha\beta} - \frac{1}{15} Q^b T^a_{\alpha\beta\gamma} \Omega^a_{\alpha\beta\gamma} - \cdots$$

The energy due to the dipole moment of *b* is $-\mu^b_\alpha F^a_\alpha(\vec{R}_{ab})$ and depends on the electric field at *b* due to *a* which, is $-\nabla^a_\alpha \phi^a(\vec{R})$. Since $T_{\alpha\beta} = \nabla_\alpha T_\beta$ & $T_{\alpha\beta\gamma} = \nabla_\alpha T_{\beta\gamma}$, *etc* we have

$$F^a_\alpha(\vec{R}) = -Q^a T^a_\alpha + T^a_{\alpha\beta}\mu^a_\beta - \frac{1}{3} T^a_{\alpha\beta\gamma}\Theta^a_{\beta\gamma} + \frac{1}{15} T^a_{\alpha\beta\gamma\delta}\Omega^a_{\beta\gamma\delta} + \cdots$$

resulting in

$$-\mu^b_\alpha F^a_\alpha(\vec{R}) = Q^a \mu^b_\alpha T^a_\alpha - T^a_{\alpha\beta}\mu^b_\alpha \mu^a_\beta + \frac{1}{3} T^a_{\alpha\beta\gamma}\mu^b_\alpha \Theta^a_{\beta\gamma} - \frac{1}{15} T^a_{\alpha\beta\gamma\delta}\mu^b_\alpha \Omega^a_{\beta\gamma\delta} + \cdots$$

The electric field gradient, $F^a_{\alpha\beta}(\vec{R})$ is obtained by applying ∇^a_α to $F^a_\beta(\vec{R})$ which simply bumps each *T* tensor up a notch.

$$\nabla^a_\alpha F^a_\beta(\vec{R}) = F^a_{\alpha\beta} = -Q^a T^a_{\alpha\beta} + T^a_{\alpha\beta\gamma}\mu^a_\gamma - \frac{1}{3} T^a_{\alpha\beta\gamma\delta}\Theta^a_{\gamma\delta} + \frac{1}{15} T^a_{\alpha\beta\gamma\delta\varepsilon}\Omega^a_{\gamma\delta\varepsilon} + \cdots$$

and so the energy due to the quadrupole moment of *a* is

$$-\frac{1}{3}\Theta^b_{\alpha\beta}F^a_{\alpha\beta}(\vec{R})=\frac{1}{3}Q^a\Theta^b_{\alpha\beta}T^a_{\alpha\beta}-\frac{1}{3}T^a_{\alpha\beta\gamma}\Theta^b_{\alpha\beta}\mu^a_\gamma+\frac{1}{9}T^a_{\alpha\beta\gamma\delta}\Theta^b_{\alpha\beta}\Theta^a_{\gamma\delta}-\frac{1}{45}T^a_{\alpha\beta\gamma\delta\varepsilon}\Theta^b_{\alpha\beta}\Omega^a_{\gamma\delta\varepsilon}+\cdots$$

The first two terms of the octupole contribution are

$$-\frac{1}{15}\Omega^b_{\alpha\beta\gamma}F^a_{\alpha\beta\gamma}=-\frac{1}{15}\Omega^b_{\alpha\beta\gamma}\left(-Q^aT^a_{\alpha\beta\gamma}+T^a_{\alpha\beta\gamma\delta}\mu^a_\delta-\cdots\right)$$

The total interaction energy becomes

$$\begin{aligned}
V_{ab}&=\frac{Q^aQ^b}{R}\\
&+T^a_\alpha\left(Q^b\mu^a_\alpha-Q^a\mu^b_\alpha\right)\\
&+\frac{1}{3}T^a_{\alpha\beta}\left(Q^b\Theta^a_{\alpha\beta}-3\mu^b_\alpha\mu^a_\beta+Q^a\Theta^b_{\alpha\beta}\right)\\
&+\frac{1}{15}T^a_{\alpha\beta\gamma}\left(-Q^b\Omega^a_{\alpha\beta\gamma}+5\mu^b_\alpha\Theta^a_{\beta\gamma}-5\mu^a_\alpha\Theta^b_{\beta\gamma}+Q^a\Omega^b_{\alpha\beta\gamma}\right)\\
&+\cdots
\end{aligned}$$

Note that the terms are ordered according to the distance dependence of the interaction energy. $T^a_\alpha : \frac{1}{R^2}, T^a_{\alpha\beta} : \frac{1}{R^3}, T^a_{\alpha\beta\gamma} : \frac{1}{R^4}$, etc. Note also the asymmetry in the signs with which moments on *a* and *b* enter the equations.

In there present form these equations are very general and simpler forms appropriate for special cases are often more useful in practice.

Some special cases

a. Point dipole at the origin, pointed along the +z axis interacting with a charge at the terminus of a vector $\vec{R}$.

The charge - dipole term is

$$V_{ab}=T^a_\alpha\left(Q^b\mu^a_\alpha-Q^a\mu^b_\alpha\right)$$

In the derivation of V_{ab}, distribution a was centered at the origin while b was at the terminus of the vector $\vec{R}$ so in this example we identify the dipole with *a* and the charge with *b*.

$$V_{ab}=T^a_\alpha Q\mu_\alpha=T^a_zQ\mu=-\frac{Q\mu\cos(\theta)}{R^2}$$

b. Point dipole at the origin, pointed along the +z axis interacting with a dipole in the yz plane. Let the dipole in the plane have the components μ_z^b & μ_y^b. The dipole-dipole interaction term is

$$V_{ab} = -T_{\alpha\beta}^a \mu_\alpha^a \mu_\beta^b = -T_{z\beta}^a \mu_z^a \mu_\beta^b = -\mu_z^a \left(T_{zz}^a \mu_z^b + T_{zy}^a \mu_y^b \right)$$

Since $T_{zz}^a = \frac{3z^2 - R^2}{R^5} = \frac{3\cos^2(\theta) - 1}{R^3}$ and $T_{zy}^a = \frac{3zy}{R^5} = \frac{3\sin(\theta)\cos(\theta)}{R^3}$ we have

$$V_{ab} = -\frac{\mu_z^a}{R^3} \left((3\cos^2(\theta) - 1)\mu_z^b + 3\sin(\theta)\cos(\theta)\mu_y^b \right)$$

Note the special cases:

$$\theta = 0 \quad then\ V_{ab} = -\frac{2\mu_z^a \mu_z^b}{R^3}$$

$$\theta = 90 \quad then\ \ V_{ab} = +\frac{\mu_z^a \mu_z^b}{R^3}$$

$$\theta = 180 \quad then\ \ V_{ab} = -\frac{2\mu_z^a \mu_z^b}{R^3}$$

c. Linear Quadrupole at the origin and a charge at terminus of vector $\vec{R}$

$$V_{ab} = \frac{1}{3} T_{\alpha\beta}^a Q^b \Theta_{\alpha\beta}^a = \frac{1}{3} Q^b \left(T_{xx}^a \Theta_{xx}^a + T_{yy}^a \Theta_{yy}^a + T_{zz}^a \Theta_{zz}^a \right)$$

since the quadrupole is linear and its trace is zero we have

$\Theta_{xx}^a = \Theta_{yy}^a = -\frac{1}{2}\Theta_{zz}^a$ and so

$$V_{ab} = \frac{1}{2} T_{zz}^a Q^b \Theta_{zz}^a = \frac{1}{2} Q^b \Theta_{zz}^a \frac{\left(3\cos^2\theta - 1\right)}{R^3}$$