APPENDIX-A

COULOMB INTERACTION ENERGY BETWEEN TWO DEFORMED AND ORIENTED NUCLEI

The derivation of Coulomb interaction energy consists of reducing \[ E_c(i\delta_1\delta_2,\gamma_1,\gamma_2,\theta_1,\phi_1,\psi_1;\beta_2,\phi_2,\psi_2) = \sum_{\eta_i,\eta_2,\eta_1} \frac{\eta_i!\eta_2!\eta_1!\eta_{i+1}!\eta_{i+1}!}{\eta_i!\eta_{i+1}!\eta_{i+1}!\eta_{i+1}!} \left( \frac{\eta_i+1}{\eta_{i+1}} \right)^{\frac{1}{2}} \right) \]

\[ \times \frac{D_{\eta_1}^{\eta_2}(\eta_1,\phi_1,\psi_1)^* \cdot D_{\eta_i}^{\eta_i}(\eta_i,\phi_i,\psi_i)_{m_i,m_2}}{R_{\eta_i+1}^{\eta_i+1}} \]

(A.1)

Here \( Q(i)_{\eta_i}^{n_i} \) is the multiple moment of the charge distributions \((i = 1 \text{ and } 2)\), calculated with respect to a body-fixed coordinate system \( x', y', z' \), and \( D^\eta_i(\theta_1, \phi_1, \psi_1)_{m_i,m} \) are the representation coefficients of the three-dimensional rotation group (the D-functions). The asterisk denotes the complex conjugation. The orientation of the body-fixed system \( x', y', z' \) with respect to the space-fixed system \( x', y', z' \) is specified by the three Euler Angles \( \theta_1, \phi_1, \psi_1 \) as shown in
Fig. 5. The distance between the origins of the co-ordinate systems $\mathbf{x}_{k}, \mathbf{y}_{k}, \mathbf{z}_{k}$ is denoted by $R$.

For uniformly charged spheroidal charge distributions we choose the body-fixed $\mathbf{z}_{i}$ axes to lie along the symmetry axes of spheroid $i$. Then, because of azimuthal symmetry about the $\mathbf{z}_{i}$ axes, $\tilde{Q}(i)\, n_{i}^{m_{i}} = 0$ for $m_{i} \neq 0$. For $m_{i} = 0$, one can show [56] that

$$
\tilde{Q}(i)\, n_{i}^{m_{i}} = 0 \quad \text{for } m_{i} \neq 0 \\
\frac{3 \, Z_{i} \epsilon (a_{i} - b_{i})^{3/2} \, n_{i}^{m_{i}}}{(n_{i} + 1)(n_{i} + 3)} \quad \text{for } m_{i} = 0
$$

where $Z_{i} \epsilon$ is total charge of the spheroid $i$, $a_{i}$ and $b_{i}$ being the semi-major and semi-minor axes, related to the deformation parameter $\beta_{i} = a_{i}/b_{i}$ through the following volume conservation relation

$$
a_{i} = \gamma_{i} A_{i}^{\frac{1}{3}} b_{i}^{\frac{2}{3}}; \quad b_{i} = \gamma_{i} A_{i}^{\frac{1}{3}} b_{i}^{-\frac{2}{3}}
$$

Since $\tilde{Q}(i)\, n_{i}^{m_{i}} = 0$ for $m_{i} \neq 0$ and $\tilde{Q}(i)\, n_{i}^{m_{i}} = 0$ for $m_{i} = 0$, the fivefold summation reduces to a triple summation and the $n_{i}^{m}$ summations need be taken over even integers only. Defining $n_{i} = 2j$ and $n_{i} = 2k$, the interaction energy becomes

$$
E_{C}(\beta_{i}, \theta_{i}, \phi_{i}, \psi_{i}) = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{3}{k^{2j + 2k + 1}(2j+1)(2j+3)(2k+1)(2k+3)} \\
\chi \sum_{m=-m_{i}}^{m_{i}} \left[ (-1)^{m}(2j+2k)! \, D^{(2j)}(\theta_{i}, \phi_{i}, \psi_{i})_{0,m} \, D^{(2k)}(\theta_{i}, \phi_{i}, \psi_{i})_{0,m} \right]^{1/2}
$$

(A.4)
where \( m' \) is the minimum of \( 2j \) and \( 2k \). Substituting for the \( D \) functions in terms of the spherical harmonics as

\[
D(\theta, \phi, \psi)_{0,m} = \left( \frac{4\pi}{2n+1} \right)^{\frac{1}{2}} Y_n^m(\theta, \phi)_{0,m}
\]

(A.5)

with

\[
Y_n^m(\theta, \phi) = i^{|m|} \frac{\Gamma(2n+1) \Gamma(n-|m|)!}{4\pi \Gamma(n+|m|)!} P_n^m(\cos \theta) e^{im\phi}
\]

(A.6)

where \( \theta \) and \( \phi \) are the usual polar angles specifying the orientation of the body fixed \( z \) axes with respect to the space-fixed \( z \) axes, Eq (A.4) becomes

\[
E_c(\beta_1, \theta_1, \phi_1; \beta_2, \theta_2, \phi_2) = \frac{Z_1 Z_2 e^2}{R} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{3}{(2j+1)(2j+3)} \frac{3}{(2k+1)(2k+3)}
\]

\[
\times \left( \frac{a_1^2 - b_1^2}{R^2} \right)^j \left( \frac{a_2^2 - b_2^2}{R^2} \right)^k
\]

\[
\times \sum_{m=-m'}^{m'} (-1)^m (2j+2k)! P_{j,j}^m(\cos \theta_1) P_{2k}^m(\cos \theta_2) e^{im(\phi_1-\phi_2)}
\]

(A.7)

The imaginary quantities and absolute values can be eliminated by writing (A.7) as follows:

\[
E_c(\beta_1, \theta_1; \beta_2, \theta_2, \phi) = \frac{Z_1 Z_2 e^2}{R} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{3}{(2j+1)(2j+3)} \frac{3}{(2k+1)(2k+3)} (2j+2k)!
\]

\[
\times \left( \frac{a_1^2 - b_1^2}{R^2} \right)^j \left( \frac{a_2^2 - b_2^2}{R^2} \right)^k
\]

\[
\times \left[ \frac{P_{j,j}^m(\cos \theta_1) P_{2k}^m(\cos \theta_2)}{(2j)! (2k)!} + 2 \sum_{m_1}^{m'} (-1)^m P_{j,j}^m(\cos \theta_1) P_{2k}^m(\cos \theta_2) \cos m_1 \phi \right]
\]

(A.8)
where \( \phi = \phi_1 - \phi_2 \) (Note that when either \( j \) or \( k \) is zero, the summation over \( m \) does not occur). Defining 

\[
\delta_{l}^{2} = \left( \frac{a_{l}^{2} - b_{l}^{2}}{R^{2}} \right)
\]

equation (A.8) can now be written as

\[
E_{c}(\beta_{1}, \theta_{1}; \beta_{2}, \theta_{2}; \phi) = \frac{Z_{l}Z_{l}e^{\delta}}{R} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{3}{(2j+1)(2j+3)} \frac{3}{(2k+1)(2k+3)}
\]

\[
\times \left[ \frac{(2j+2k)!}{(2j)!(2k)!} \delta_{l}^{2j} \delta_{l}^{-2k} \right]
\]

\[
\times \left[ \frac{p_{2j}^{m_{j}}(\cos \theta_{1})p_{2k}^{m_{k}}(\cos \theta_{2}) + 2}{(2j+m)!(2k+m)!} \sum_{m=1}^{m_{j}} \frac{(-1)^{m_{j}}(z_{j})!}{(z_{j}+m)!} \frac{m_{j}^{m_{j}}(\cos \theta_{1})(z_{k})!}{(z_{k}+m)!} \frac{m_{k}^{m_{k}}(\cos \theta_{2})}{\cos m\phi} \right]
\]

(A.9)

When either \( j=0 \) or \( k=0 \) in this result, the single remaining summation can be performed explicitly. It is thus convenient to write (A.9) as

\[
E_{c}(\beta_{1}, \theta_{1}; \beta_{2}, \theta_{2}; \phi) = \frac{Z_{l}Z_{l}e^{\delta}}{R} \sum_{\eta_{l}=0}^{\infty} \frac{3}{(2\eta_{l}+1)(2\eta_{l}+3)} (2\eta_{l}^{2} + 3) \]

(A.10)

where

\[
\delta_{l}^{2} = \sum_{\eta_{l}=0}^{\infty} \frac{3}{(2\eta_{l}+1)(2\eta_{l}+3)}
\]

(A.11)

and

\[
\delta_{l}^{2} = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \frac{3}{(2j+1)(2j+3)} \frac{3}{(2k+1)(2k+3)}
\]

(A.12)

The equations can be further reduced [57] to write for prolate and oblate spheroids separately. For the prolate spheroid,
where  
\[ q_i^2 = \frac{1}{2} \left\{ 1 + \delta_i^2 + \left[ 1 - 2 \left( 2 \cos^2 \theta_i - 1 \right) \delta_i^2 + \frac{3}{4} \right]^{1/2} \right\} \]  
(A.13)  
and  
\[ h_i^2 = \frac{1}{2} \left\{ 1 - \delta_i^2 + \left[ 1 - 2 \left( 2 \cos^2 \theta_i - 1 \right) \delta_i^2 + \frac{3}{4} \right]^{1/2} \right\} \]  
and for an oblate spheroid  
\[ S_{ij}^2 (\phi, \theta) = \left[ \frac{3}{2 \omega_i^2} + \left( \frac{9}{4} \cos^2 \theta_i - \frac{3}{4} \right) \frac{1}{\omega_i^2} \right] \tan^{-1} \left( \frac{\omega_i}{g_i} \right) - \frac{3 \cos^2 \theta_i}{2 \omega_i^2 h_i^2} + \frac{3 g_i^2 \sin^2 \theta_i}{4 \omega_i^2 h_i^2} \]  
(A.14)  
where \( \omega_i^2 = \delta_i^2 \).  

The last term \( S \) of equation (A.10), for the symmetry axes of the spheroids lying in the same plane (\( \phi = 0^\circ \)) and parallel to each other (\( \theta_1 = \theta_2 = \theta \)), reduces to  
\[ S_{ij} = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} \frac{3}{(2j+1)(2j+3)} \frac{3}{(2k+1)(2k+3)} \frac{(2j+2k)!}{(2j+1)(2j+3)(2k)!} \Delta_j^j \Delta_k^k \frac{p_i^j}{2j+2k} \]  
(A.15)  

Since the quadrupole interaction term is the most important of the multipole terms of the charge distribution, the correction term \( S \) for such interaction (\( j = k = 1 \)) reduces to  
\[ S_{ij} (\phi, \theta) = \frac{8}{300} \Delta_i^2 \Delta_j^2 \left( 9 + 20 \cos 2\theta + 35 \cos 4\theta \right) \]  
(A.16)  
for prolate as well as oblate spheroids.