

Task 1. Dipole Moments. (70 points). You are given the Cartesian expression for the dipole moment \vec{p} of a charge distribution $\rho = \rho(\vec{r})$, which is $\vec{p} = \int d^3r \vec{r} \rho(\vec{r})$. Furthermore, you are given the general expression for multipole moments $q_{\ell m}$ in spherical coordinates, $q_{\ell m} = \int \rho(\vec{r}) r^\ell Y_{\ell m}^*(\theta, \varphi) d^3r$.

(a.) Based on the **three** conversion formulas (which you can take for granted),

$$q_{11} = -\sqrt{\frac{3}{8\pi}} (\rho_x - i\rho_y), \quad q_{1-1} = \sqrt{\frac{3}{8\pi}} (\rho_x + i\rho_y), \quad q_{10} = \sqrt{\frac{3}{4\pi}} \rho_z. \quad (1)$$

determine the entries of the conversion matrix $\mathbb{C} = (C_{ij})_{i,j}$ with $i = 1, 2, 3$ and $j = 1, 2, 3$, i.e., determine the entries C_{ij} in the following matrix

$$\begin{pmatrix} q_{11} \\ q_{1-1} \\ q_{10} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix} \cdot \begin{pmatrix} \rho_x \\ \rho_y \\ \rho_z \end{pmatrix}. \quad (2)$$

(b.) Determine the block structure of \mathbb{C} . Based on the block structure, calculate the inverse \mathbb{C}^{-1} of the conversion matrix. Determine which four elements of \mathbb{C}^{-1} are zero.

Task 2. Quadrupole Moments. (70 points). You are given the Cartesian components of the quadrupole tensor ($\vec{r} = \sum_{i=1}^3 x_i \hat{e}_i$),

$$Q_{ij} = \int d^3r (3x_i x_j - \delta_{ij} r^2) \rho(\vec{r}), \quad (3)$$

with $i = 1, 2, 3$ and $j = 1, 2, 3$. The element $q_{(\ell=2)(m=-2)}$ of the in spherical coordinates is

$$q_{22} = \int \rho(\vec{r}) r^2 Y_{2-2}^*(\theta, \varphi) d^3r, \quad \text{where } Y_{22}(\theta, \varphi) = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{-2i\varphi}. \quad (4)$$

Your task is to express the spherical tensor element q_{22} in terms of the elements of the Cartesian Q_{ij} tensor. Show your work! Show every intermediate step with diligence! **Hint:** You might encounter a decomposition of the form $q_{22} = \mathcal{A} Q_{11} + \mathcal{B} Q_{22} + \mathcal{C} Q_{12}$, with the coefficients \mathcal{A} , \mathcal{B} and \mathcal{C} to be determined. At some point in your calculations, you might use the (somewhat trivial) identity

$$x^2 - y^2 = \frac{2x^2 - y^2 - z^2}{3} - \frac{2y^2 - x^2 - z^2}{3}. \quad (5)$$

Task 3. Dipole–Dipole Interactions. (60 points). The dipole term in Eq. (5.122) of the lecture notes describes the interaction energy W of a local charge distribution with dipole moment \vec{p}_1 , located at the origin, with an external electric field $\vec{E}_{\text{ext}}(\vec{0})$,

$$W_{\text{dipole}} = -\vec{E}_{\text{ext}}(\vec{0}) \cdot \vec{p}_1. \quad (6)$$

Now, assume that $\vec{E}_{\text{ext}}(\vec{0})$ is the external field, observed at the observation point $\vec{r} = \vec{0}$, generated by a dipole \vec{p}_2 located at point \vec{R} . **Hence, derive the dipole-dipole interaction energy between dipoles \vec{p}_1 and \vec{p}_2 a distance \vec{R} apart. Include a drawing!** Show your work! Show every intermediate step with diligence!

Hint: First, write the *electrostatic potential* (not field!) generated by \vec{p}_2 at the observation point \vec{r} . Finally, you will set $\vec{r} = \vec{0}$, but not just yet. Your expression might contain terms $\vec{r} - \vec{R}$. Then, differentiate the electrostatic potential with respect to \vec{r} (not \vec{R} !), to get the electric field from the potential at the point \vec{r} . As a last step, set $\vec{r} = \vec{0}$. Your result might be *not equal to, but proportional to*

$$W_{\text{dipole}} \propto \frac{\vec{p}_1 \cdot \vec{p}_2 - 3(\hat{R} \cdot \vec{p}_1)(\hat{R} \cdot \vec{p}_2)}{R^3}, \quad \hat{R} = \frac{\vec{R}}{|\vec{R}|} = \frac{\vec{R}}{R}. \quad (7)$$