Problem Assignment # 10 04/01/2021
due 04/08/2021

2.3.1. **Quadrupole moments (continued)**

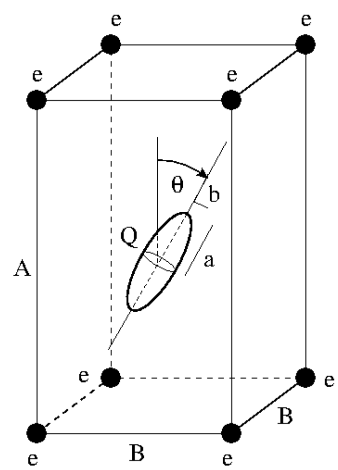
This is a continuation of Problem #2.3.1.

e) Consider the homogeneously charged ellipsoid from part c) and calculate the quadrupole moments Q_{2m} as defined in ch.2 §3.5.

(3 points)

2.3.7. **Electrostatic interaction II: Quadrupole in an external electric field**

Consider the following classical model for a nuclear quadrupole moment in a crystal lattice: A rectangular parallelepiped (height A, length and width B) carries a charge e at each of its eight corners. At the center of the parallelepiped is a homogeneously charged spheroid (charge Q, semi-axes a and b). The symmetry axis of the spheroid forms an angle θ with the A-axis of the parallelepiped. The center of the spheroid is fixed, but the angle θ can vary. Let $A \gg a$, $B \gg b$.



a) Calculate the electrostatic interaction energy U of this system to quadrupolar order. Show that U can be expressed in terms of e, the lattice constants A and B, and the quadrupole moment Q_{33} of the spheroid in the coordinate system of the lattice.

b) Calculate the quadrupole moment Q'_{33} of the spheroid in its principal-axes system, and then calculate Q_{33} by transforming into the lattice system. Express U as a function of the angle θ.

hint: In general, lining up the principal-axes systems would require three Euler angles. However, due to the symmetries of the problem Q'_{33} and Q_{33} in the present case are related by only one angle, viz., θ.

c) Find the equilibrium positions of the spheroid. Make sure to distinguish the cases of prolate and oblate spheroids ($a > b$ and $a < b$, respectively), as well as between the cases $A > B$ and $A < B$.

(15 points)

2.3.8. **Electric charges in an external field**

Consider a static electric charge distribution $\rho(\boldsymbol{x})$ subject to a static potential $\varphi(\boldsymbol{x})$. Consider the force $\boldsymbol{F}_{\text{el}}$ on the charge distribution and show that $\boldsymbol{F}_{\text{el}} = -\boldsymbol{\nabla} U$, with U the electrostatic energy calculated in ch.3 §3.6. In particular, convince yourself that the dipole term in the multipole expansion of U gives the correct potential energy for an electric dipole moment $\boldsymbol{d}$ in an electric field $\boldsymbol{E}$.

(3 points)

2.3.1.) e.)

$$\underline{Q_{20}} = \sqrt{\frac{4\pi}{5}} \int_0^\infty dr\, r^4 \int d\Omega\, \rho(r,\Omega) \sqrt{\frac{5}{4\pi}}\, \frac{1}{2}(3\eta^2-1)$$

$$= \frac{1}{2}\int d\vec{x}\, \rho(\vec{x})\,(3z^2-r^2) = \underline{D_{33}}$$

(1)

$$\underline{Q_{2,\pm1}} \propto \int d\Omega\, \underbrace{\rho(r,\Omega)}_{\text{even}}\, \underbrace{P_2^{\pm1}(\eta)}_{\text{odd}} = \underline{0} \text{ by symmetry}$$

odd fct. of η

(1)

$$\underline{Q_{22}} = \sqrt{\frac{4\pi}{5}} \int_0^\infty dr\, r^4 \int d\Omega\, \rho(r,\Omega) \sqrt{\frac{5}{4\pi}}\, \frac{1}{\sqrt{4!}}\, e^{2i\varphi}\, 3(1-\eta^2)$$

$$= \frac{3}{\sqrt{24}} \int d\vec{x}\, \rho(\vec{x})\, r^2 (1-\eta^2)(\cos 2\varphi + i \sin 2\varphi)$$

$$= \frac{3}{\sqrt{24}} \int d\vec{x}\, \rho(\vec{x})\, r^2 \sin^2\vartheta\, (\cos^2\varphi - \sin^2\varphi) + \frac{3i}{\sqrt{24}} \int d\vec{x}\, \underbrace{\rho(\vec{x})\, r^2 \sin^2\vartheta}_{\text{even}}\, \underbrace{\sin 2\varphi}_{\text{odd}}$$

odd fct. of φ $\to 0$

$$= \frac{3}{\sqrt{24}} \int d\vec{x}\, \rho(\vec{x})\, r^2 (\sin^2\vartheta \cos^2\varphi - \sin^2\vartheta \sin^2\varphi)$$

$x = r \sin\vartheta \cos\varphi$

$y = r \sin\vartheta \sin\varphi$ $\Big\} \leadsto x^2 - y^2 = r^2 \sin^2\vartheta (\cos^2\varphi - \sin^2\varphi)$

$z = r \cos\vartheta$

$$= \frac{3}{2\sqrt{6}} \int d\vec{x}\, \rho(\vec{x})\, (x^2-y^2)$$

$$= \frac{3}{2\sqrt{6}} \int d\vec{x}\, \rho(\vec{x}) \left[(2x^2-y^2-z^2) - (2y^2-x^2-z^2)\right] \frac{1}{3}$$

$$= \underline{\frac{1}{\sqrt{6}} (D_{11} - D_{22})}$$

$$\underline{Q_{2,-2}} = \sqrt{\frac{4\pi}{5}} \int_0^\infty dr\, r^4 \int d\Omega\, \rho(r,\Omega) \sqrt{\frac{5}{4\pi}}\, \sqrt{4!}\, e^{-2i\varphi}\, \frac{1}{8}(1-\eta^2) = \underline{Q_{22}}$$

(1)

2.3.4.) a) cf. 3.6 → Consider the potential due to the 8 charges:

$$\varphi(\vec{x}) = e\sum_{\alpha=1}^{8} \frac{1}{|\vec{x}-\vec{\xi}^{(\alpha)}|} \quad \text{where} \quad \vec{\xi}^{(\alpha)} = \frac{1}{2}\begin{pmatrix} \pm a \\ \pm a \\ \pm A \end{pmatrix}$$

We need

(1) $$\underline{\varphi_0} = \varphi(\vec{x}=0) = e\sum_{\alpha=1}^{8}\frac{1}{|\vec{\xi}^{(\alpha)}|} = e\,\frac{8}{\sqrt{A^2/4+2a^2/4}} = \underline{\frac{16e}{\sqrt{A^2+2a^2}}}$$

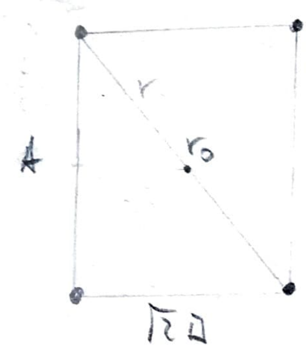
(1) $$\vec{E} = -\vec{\nabla}\varphi(\vec{x}=0) = \sum_{\alpha=1}^{8}\frac{-\vec{\xi}^{(\alpha)}}{|\vec{\xi}^{(\alpha)}|^3} = 0 \quad \text{by symmetry}$$

(1) $$\varphi_{ij} = \frac{\partial^2}{\partial x_i \partial x_j}\varphi\Big|_{\vec{x}=0} = \begin{pmatrix} \varphi & 0 & 0 \\ 0 & \varphi & 0 \\ 0 & 0 & -2\varphi \end{pmatrix} \quad \text{by symmetry (see Problem 3.5e!)}$$

where

(1) $$\underline{\varphi} = \varphi_{11} = \frac{\partial^2}{\partial x^2}\Big|_{\vec{x}=0} e\sum_{\alpha=1}^{8}\frac{1}{|\vec{x}-\vec{\xi}^{(\alpha)}|} = e\left(\frac{3(\xi_1^{(\alpha)})^2}{|\vec{\xi}^{(\alpha)}|^5} - \frac{1}{|\vec{\xi}^{(\alpha)}|^3}\right)$$

Define $r_0 := \sqrt{A^2+2a^2} \rightarrow |\vec{\xi}^{(\alpha)}| = \frac{1}{2}r_0$



$$\rightarrow \underline{\varphi_0 = \frac{16e}{r_0}}$$

$$\underline{\varphi} = e\left(\frac{3a^2/4}{(r_0/2)^5} - \frac{1}{(r_0/2)^3}\right)$$

(1) $$= e\frac{1}{r_0^5}\left(\frac{3}{4}a^2\cdot 8\cdot 4 - 8r_0^2\right) = \frac{8e}{r_0^5}\left(3a^2 - A^2 - 2a^2\right) = \underline{\frac{8e}{r_0^5}(a^2-A^2)}$$

$$\rightarrow \underline{U} = \varphi_0 Q + \frac{1}{3}\left(\varphi Q_{11} + \varphi Q_{22} - 2\varphi Q_{33}\right)$$

$$= \varphi_0 Q + \frac{1}{3}\varphi\left(Q_{11}+Q_{22}-2Q_{33}\right)$$

(1) $\sum_i Q_{ii} = 0 \rightsquigarrow$ $$= \underline{\underline{\varphi_0 Q - \varphi Q_{33}}}$$

remark: then Q_{33} is the quadrupole moment of the spheroid in the lattice coordinate system!

b) In the principal-axes system of the spheroid the quadrupole tensor has the form

$$Q'_{ij} = \begin{pmatrix} q & 0 & 0 \\ 0 & q & 0 \\ 0 & 0 & -2q \end{pmatrix}$$

(1)

Transform to the lattice system by means of rotation matrices (elements of SO(3)) D:

(1) $$Q_{ij} = \sum_{k,l} D_{ik} Q'_{kl} D_{jl}$$

$$\Rightarrow Q_{33} = D_{31} Q'_{11} D_{31} + D_{32} Q'_{22} D_{32} + D_{33} Q'_{33} D_{33}$$

$$= q (D_{31})^2 + q (D_{32})^2 - 2q (D_{33})^2$$

$$= q \left[(D_{31})^2 + (D_{32})^2 - 2 (D_{33})^2 \right]$$

(1)

(1) Now D_{ij} is an orthogonal trafo $\Rightarrow$ $D_{31}^2 + D_{32}^2 + D_{33}^2 = 1$

(1) and D must align the z'-axis with the z-axis $\Rightarrow$ $D_{33} = \cos\theta$

$$\Rightarrow Q_{33} = q \left[1 - D_{33}^2 - 2 D_{33}^2 \right] = q \left[1 - 3\cos^2\theta \right]$$

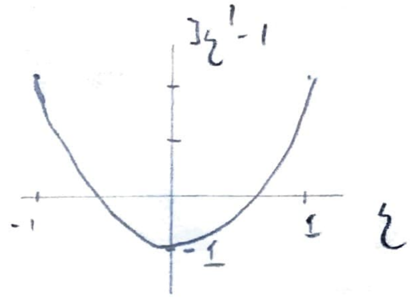
Finally, Problem 20 with $q = \frac{Q}{10}(b^2 - a^2)$

$$\Rightarrow U = \varphi_0 Q - \frac{8e}{r_0^5} (B^2 - A^2)\, q\, (1 - 3\cos^2\theta)$$

(1) $$= \varphi_0 Q + \frac{8e}{r_0^5} \frac{Q}{10} (A^2 - B^2)(a^2 - b^2)(3\cos^2\theta - 1)$$

c) $3\eta^2-1$ is minimal for $\eta=0$

$\Leftrightarrow \vartheta=\pi/2$



maximal for $\eta=\pm 1$

$\Leftrightarrow \vartheta = 0,\pi$

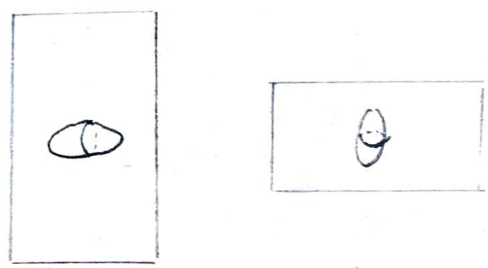
let $eQ>0$ → U is minimal for

$\vartheta=\frac{\pi}{2}$ if $(A^2-B^2)(a^2-b^2)>0$

(1) $\vartheta=0$ if $(A^2-B^2)(a^2-b^2)<0$

prolate spheroid $(a>b)$:

(cigar)



(1)

oblate $(a<b)$: flips the two cases

(disc)

(1) $eQ<0$: Flips the two cases again.

2.3.8.) cf 2 §§ 2.5, 2.5a → The force on a single charge is $\vec{\nabla} e \varphi(\vec{x})$

→ The force on $\rho(\vec{x}) = \sum_\alpha e_\alpha \delta(\vec{x}-\vec{x}_\alpha)$ is

(1) $$\vec{F}_{el} = -\sum_\alpha e_\alpha \vec{\nabla}\varphi(\vec{x}) = -\int d\vec{x}\, \rho(\vec{x})\, \vec{\nabla}\varphi(\vec{x}) \overset{\text{cf 2 §2.4}}{=} +\int d\vec{x}\, \rho(\vec{x})\, \vec{E}(\vec{x})$$

Now expand as in cl 3 § 3.6:

$$F_{el}^i = -\int d\vec{x}\, \rho(\vec{x}) \left[\partial_i \varphi\big|_{x=0} + x_j \partial_j \partial_i \varphi\big|_{x=0} + \dots \right]$$

$$= -Q\, \partial_i \varphi - (\partial_i \partial_j \varphi)_{\vec{x}=0} \int d\vec{x}\, x_j\, \rho(\vec{x}) + \dots \qquad \underline{Q = \int d\vec{x}\, \rho(\vec{x})}$$

$\partial_j \varphi = -E_j$

$$= -Q(\partial_i \varphi)_{\vec{x}=0} + (\partial_i E_j)_{\vec{x}=0}\, d_j + \dots \qquad \underline{\vec{d} = \int d\vec{x}\, \vec{x}\, \rho(\vec{x})}$$

$$= -\partial_i \Big|_{\vec{x}=0} \left[Q\varphi - \vec{E}\cdot\vec{d} + \dots \right]$$

(1) → $\underline{\underline{\vec{F}_{el} = -(\vec{\nabla} U)_{\vec{x}=0}}}$ with $U(\vec{x}) = Q\varphi(\vec{x}) - \vec{d}\cdot\vec{E}(\vec{x})$ from cl 3 § 3.6 and $\vec{x}$ is put to zero after calculating the gradient.

In particular, the dipole term in the electrostatic energy,

$$\underline{\underline{U_{dipole} = -\vec{E}\cdot\vec{d}}}$$

(1) which describes the potential energy of a fixed electric dipole $\vec{d}$ in an electric field $\vec{E}$.