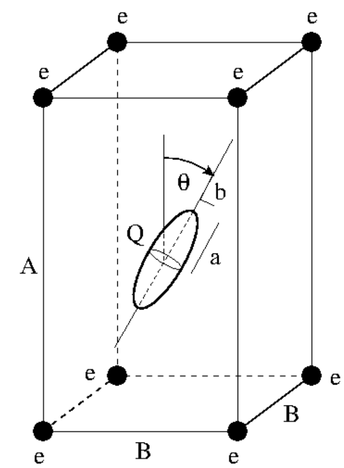
2.3.8. **Electrostatic interaction III: Quadrupole in an external electric field**

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

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

We need

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

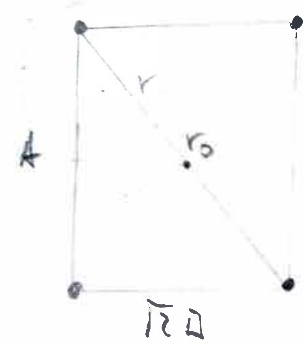
1 $$\vec{E} = -\vec{\nabla}\varphi(\vec{x}=0) = \sum_{\alpha=1}^{8} \frac{-\vec{\xi}^{(\alpha)}}{|\vec{\xi}^{(\alpha)}|^3} = 0 \quad \text{by symmetry}$$

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



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

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

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

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

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

1 $\sum_i Q_{ii} = 0 \quad \rightarrow$ $$= \underline{\underline{\varphi_0 Q - \varphi Q_{33}}}$$

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

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

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

$$Q_{ij} = \sum_{n,m} D_{in} Q'_{nm} D_{jm}$$

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

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

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

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

and D must align the z'-axis with the z-axis $\rightarrow$ $D_{33} = \cos\vartheta$

$$\rightarrow \quad Q_{33} = q \left[1 - D_{33}^2 - 2 D_{33}^2 \right] = q \left[1 - 3\cos^2\vartheta \right]$$

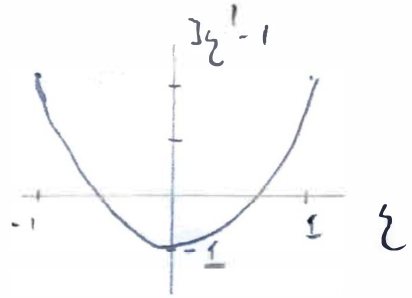
Finally, Problem 20 with $q = \frac{Q}{10}(b^2 - a^2)$

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

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

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

$\Leftrightarrow \vartheta = \pi/2$



maximal for $\eta = \pm 1$

$\Leftrightarrow \vartheta = 0, \pi$

let $eQ > 0$ $\rightarrow$ U is minimal for

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

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

1

prolate spheroid $(a > b)$

(cigar)

1

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

(disc)

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