Problem Assignment # 8 03/06/2024
due 03/13/2024

2.3.5. **Field due to distant charges**

Consider the electric field generated by a charge density $\rho(\boldsymbol{y})$ that vanishes inside a sphere with radius r_0: $\rho(\boldsymbol{y}) = 0$ for $|\boldsymbol{y}| \leq r_0$. Show that

a) If ρ is invariant under parity operations, $\rho(-\boldsymbol{y}) = \rho(\boldsymbol{y})$, then the electric field at the origin vanishes.

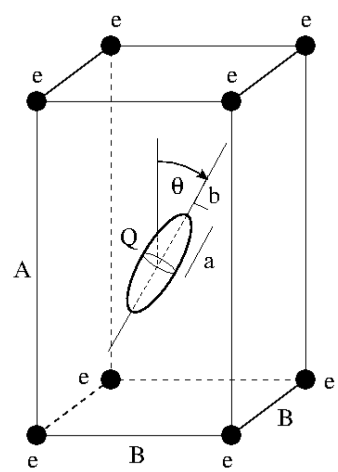
b) If $\rho(\boldsymbol{y})$ is invariant under rotations about the z-axis through multiples of an angle α with $|\alpha| < \pi$, then the field-gradient tensor at the origin has the form $\varphi_{ij}(\boldsymbol{x}=0) = \begin{pmatrix} \varphi & 0 & 0 \\ 0 & \varphi & 0 \\ 0 & 0 & -2\varphi \end{pmatrix}$

c) If $\rho(\boldsymbol{y})$ has cubic symmetry, i.e., if $\rho(\boldsymbol{y})$ is invariant under rotations through $\pi/2$ about any of the three axes x, y, and z, then the field-gradient tensor at the origin vanishes.

(6 points)

2.3.7. **Electrostatic interaction: 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)

2.3.5.)
$$\varphi(\vec{x}) = \int d\vec{\xi}\, \frac{\rho(\vec{\xi})}{|\vec{x}-\vec{\xi}|} = \varphi(\vec{x}=0) + \vec{x}\cdot\vec{\nabla}\varphi\Big|_{\vec{x}=0} + \frac{1}{2} x_i x_j \frac{\partial^2\varphi}{\partial x_i \partial x_j}\Big|_{\vec{x}=0} + \dots$$
$$=: \varphi_0 - \vec{x}\cdot\vec{E} + \frac{1}{2} x_i x_j \varphi_{ij} + \dots$$
$$\equiv \varphi_0 + \varphi_1(\vec{x}) + \varphi_2(\vec{x}) + \dots$$

a) $\rho(\vec{\xi}) = \rho(-\vec{\xi}) \rightsquigarrow \varphi(-\vec{x}) = \int d\vec{\xi}\, \frac{\rho(\vec{\xi})}{|\vec{x}+\vec{\xi}|} = \int d\vec{\xi}\, \frac{\rho(-\vec{\xi})}{|\vec{x}-\vec{\xi}|} = \varphi(\vec{x})$

1 $\rightsquigarrow$ All terms odd in $\vec{x}$ vanish, in particular $\underline{\vec{E}=0}$

b) φ_{ij} is real symmetric $\rightsquigarrow \exists$ coordinate system such that φ_{ij} is diagonal

1

$\varphi(\vec{x})$ obeys Laplace's eq. $\forall\, |\vec{x}| < r_0$

$\rightsquigarrow \sum_i \varphi_{ii} = 0$

$\rightsquigarrow \varphi_{ij}$ has the form $\varphi_{ij} = \begin{pmatrix} \varphi_+ + \varphi_- & 0 & 0 \\ 0 & \varphi_+ - \varphi_- & 0 \\ 0 & 0 & -2\varphi_+ \end{pmatrix}$

1 where $\varphi_- = \frac{1}{2}(\varphi_{11} - \varphi_{22})$

$\rightsquigarrow \underline{\varphi_2(\vec{x})} = \frac{1}{2} r^2 \sin^2\vartheta \cos^2\varphi\, (\varphi_+ + \varphi_-)$
$+ \frac{1}{2} r^2 \sin^2\vartheta \sin^2\varphi\, (\varphi_+ - \varphi_-)$
$+ \frac{1}{2} r^2 \cos^2\vartheta\, (-2\varphi_+)$

1 $= \underline{\frac{1}{2} r^2 \left[(1 - 3\cos^2\vartheta)\varphi_+ + \sin^2\vartheta \cos 2\varphi\, \varphi_- \right]}$

Rotational invariance of $\rho(\vec{\xi})$ implies rotational invariance of $\varphi(\vec{x})$, and in particular of $\varphi_2(\vec{x})$

$$\rightsquigarrow \underline{\varphi_2(r,\vartheta,\varphi+\alpha)} = \frac{1}{2}r^2\left[(1-3\cos^2\vartheta)\,\varphi_+ + \sin^2\vartheta\,\cos 2(\varphi+\alpha)\,\varphi_-\right]$$

$$\overset{!}{=} \underline{\varphi_2(r,\vartheta,\varphi)}$$

$\underline{(1)}$ $\rightsquigarrow \varphi_-\cos(2\varphi+2\alpha) = \varphi_-\cos 2\varphi \rightsquigarrow \underline{\underline{\varphi_- = 0}}$

c) cubic symmetry $\rightsquigarrow \rho(\vec{\xi})$ invariant under rotations through $\frac{\pi}{2}$ about any of the three axes x, y, z.

b) $\rightsquigarrow \varphi_- = 0$ due to invariance under rotation about z-axis

Rotation about x or y $\rightsquigarrow \vartheta \to \vartheta + \pi/2$

But invariance of $\rho(\vec{\xi})$ implies invariance of $\varphi(\vec{x})$

$$\rightsquigarrow \underline{\varphi_2(r,\vartheta+\tfrac{\pi}{2},\varphi)} = \frac{1}{2}r^2\varphi_+\left[1-3\cos^2(\vartheta+\pi/2)\right]$$

$$\overset{!}{=} \underline{\frac{1}{2}r^2\varphi_+\left[1-3\cos^2\vartheta\right]}$$

$\underline{(1)}$ $\rightsquigarrow \varphi_+\cos^2(\vartheta+\pi/2) = \varphi_+\cos^2\vartheta \rightsquigarrow \underline{\varphi_+ = 0} \rightsquigarrow \underline{\underline{\varphi_{ij} = 0}}$

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

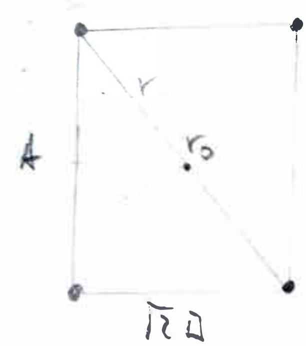
(1) $$\vec{E} = -\vec{\nabla}\varphi(\vec{x}=0) = \sum_{\alpha=1}^{8}\frac{-\vec{\xi}^{(\alpha)}}{|\vec{\xi}^{(\alpha)}|^3} = 0 \quad \text{by symmetry}$$

(1) $$\varphi_{ij} = \frac{\partial^2}{\partial x_i \partial x_j}\varphi\Big|_{\vec{x}=0} = \begin{pmatrix} \varphi & 0 & 0 \\ 0 & \varphi & 0 \\ 0 & 0 & -2\varphi \end{pmatrix}$$ by symmetry, see Problem 2.3.5 b)

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



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

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

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

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

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

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

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)

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

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

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

(1)

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

(1)

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

(1)

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

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

Finally, Problem 2.3.1 with $q = \frac{Q}{10}(b^2 - a^2)$

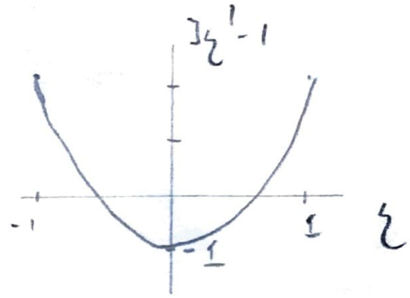
$$\Rightarrow \underline{\underline{U}} = \varphi_0 Q - \frac{8e}{r_0^5}(B^2 - A^2)\, q\, (1 - 3\cos^2\vartheta)$$

(1)

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

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

$\Leftrightarrow \vartheta=\pi/2$



maximal for $\xi=\pm 1$

$\Leftrightarrow \vartheta = 0, \pi$

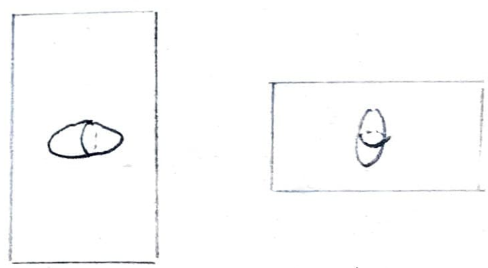
let $eQ>0$ $\rightarrow$ U is minimal for

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

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

prolate spheroid $(a>b)$:

(cigar)



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

(disc)

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