

25. **Field due to distant charges**

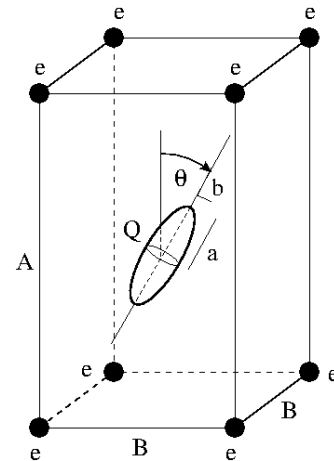
Consider the electric field generated by a charge density $\rho(\mathbf{y})$ that vanishes inside a sphere with radius r_0 : $\rho(\mathbf{y}) = 0$ for $|\mathbf{y}| \leq r_0$. Show that

- a) If ρ is invariant under parity operations, $\rho(-\mathbf{y}) = \rho(\mathbf{y})$, then the electric field at the origin vanishes.
- b) If $\rho(\mathbf{y})$ 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 $\varphi_{ij}(\mathbf{x} = 0) = \begin{pmatrix} \varphi & 0 & 0 \\ 0 & \varphi & 0 \\ 0 & 0 & -2\varphi \end{pmatrix}$
- c) If $\rho(\mathbf{y})$ has cubic symmetry, i.e., if $\rho(\mathbf{y})$ 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)

26. **Electrostatic interaction**

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)

.../over

27. Electric charges in an external field

Consider a static electric charge distribution $\rho(\mathbf{x})$ subject to a static potential $\varphi(\mathbf{x})$. Consider the force \mathbf{F}_{el} on the charge distribution and show that $\mathbf{F}_{\text{el}} = -\nabla U$, 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 \mathbf{d} in an electric field \mathbf{E} .

(3 points)

$$25.) \quad \varphi(\vec{x}) = \int d\vec{y} \frac{f(\vec{y})}{|\vec{x}-\vec{y}|} = \varphi(\vec{x}=0) + \vec{x} \cdot \vec{\nabla} \varphi \Big|_{\vec{x}=0} + \frac{1}{2} x_i x_j \frac{\partial^2 \varphi}{\partial x_i \partial x_j} \Big|_{\vec{x}=0} + \dots$$

$$\Rightarrow \varphi_0 - \vec{x} \cdot \vec{E} + \frac{1}{2} x_i x_j \varphi_{ij} + \dots$$

$$\equiv \varphi_0 + \varphi_1(\vec{x}) + \varphi_2(\vec{x}) + \dots$$

$$a) \quad f(\vec{y}) = f(-\vec{y}) \Rightarrow \varphi(-\vec{x}) = \int d\vec{y} \frac{f(\vec{y})}{|\vec{x}+\vec{y}|} = \int d\vec{y} \frac{f(-\vec{y})}{|\vec{x}-\vec{y}|} = \varphi(\vec{x})$$

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

b) φ_{ij} is real symmetric \Rightarrow \exists orthonormal basis and let φ_{ij} is diagonal

①
 $\varphi(\vec{x})$ obeys Laplace's eq. $\forall |\vec{x}| < r_0$

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

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

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

$$\begin{aligned} \Rightarrow \underline{\varphi_2(\vec{x})} &= \frac{1}{2} r^2 \hat{u}^i \partial_i \hat{u}^j \varphi (\varphi_+ + \varphi_-) \\ &+ \frac{1}{2} r^2 \hat{u}^i \partial_i \hat{u}^j \varphi (\varphi_+ - \varphi_-) \\ &+ \frac{1}{2} r^2 \hat{u}^i \partial_i (-2\varphi_+) \end{aligned}$$

$$= \underline{\underline{\frac{1}{2} r^2 [(1-\hat{u}^i \partial_i) \varphi_+ + \hat{u}^i \partial_i \hat{u}^j \varphi \varphi_-]}}$$

①
 Rotational invariance of $f(\vec{y})$ implies rotational invariance of $\varphi(\vec{x})$, and in particular of $\varphi_2(\vec{x})$

$$\begin{aligned} \rightarrow \underline{\psi_2(r, \vartheta, \varphi + \alpha)} &= \frac{1}{2} r^2 \left[(1 - \cos^2 \vartheta) \varphi_+ + \cos^2 \vartheta \cos 2(\varphi + \alpha) \varphi_- \right] \\ &\stackrel{!}{=} \underline{\psi_2(r, \vartheta, \varphi)} \end{aligned}$$

①

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

c) cubic symmetry $\rightarrow \rho(\vec{r})$ invariant under rotations through $\frac{\pi}{2}$ about any of the three axes x_i, j, z .

b) $\rightarrow \varphi_- = 0$ due to invariance under rotation about z -axis
 rotate about x or $y \rightarrow \vartheta \rightarrow \vartheta + \pi/2$

that invariance of $\rho(\vec{r})$ implies invariance of $\psi(\vec{r})$

$$\begin{aligned} \rightarrow \underline{\psi_2(r, \vartheta + \frac{\pi}{2}, \varphi)} &= \frac{1}{2} r^2 \varphi_+ \left[1 - \cos^2(\vartheta + \pi/2) \right] \\ &\stackrel{!}{=} \underline{\frac{1}{2} r^2 \varphi_+ \left[1 - \cos^2 \vartheta \right]} \end{aligned}$$

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

①

26.) a) als § 1.6 \rightarrow wieder die potential due to the 2 charges:

$$\varphi(\vec{x}) = e \sum_{k=1}^2 \frac{1}{|\vec{x} - \vec{y}^{(k)}|} \quad \text{wobei} \quad \vec{y}^{(k)} = \frac{1}{2} \begin{pmatrix} \pm a \\ \pm a \\ \pm a \end{pmatrix}$$

Wir need

$$\underline{\varphi_0} = \varphi(\vec{x}=0) = e \sum_{k=1}^2 \frac{1}{|\vec{y}^{(k)}|} = e \frac{2}{\sqrt{A^2/4 + 2A^2/4}} = \frac{16e}{\sqrt{A^2 + 2A^2}}$$

$$\underline{\vec{E}} = -\vec{\nabla} \varphi(\vec{x}=0) = \sum_{k=1}^2 \frac{-\vec{y}^{(k)}}{|\vec{y}^{(k)}|^2} = 0 \quad \text{by symmetry}$$

$$\varphi_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} \varphi \Big|_{\vec{x}=0} = \begin{pmatrix} \varphi & 0 & 0 \\ 0 & \varphi & 0 \\ 0 & 0 & -2\varphi \end{pmatrix} \quad \text{by symmetry (see Problem 15e!)}$$

wobei

$$\underline{\varphi} = \varphi_{\pm\pm} = \frac{\partial^2}{\partial x^2} \Big|_{\vec{x}=0} e \sum_{k=1}^2 \frac{1}{|\vec{x} - \vec{y}^{(k)}|} = e \left(\frac{3|\vec{y}^{(k)}|^2}{|\vec{y}^{(k)}|^5} - \frac{1}{|\vec{y}^{(k)}|^3} \right)$$

$$\text{Definiere } r_0 := \sqrt{A^2 + 2A^2} \rightarrow |\vec{y}^{(k)}| = \frac{1}{2} r_0$$

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

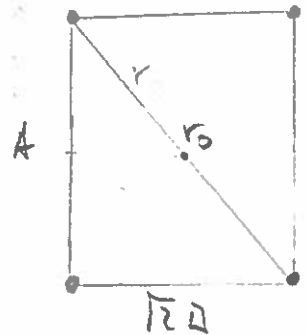
$$\underline{\varphi} = e \left(\frac{3A^2/4}{(r_0/2)^5} - \frac{1}{(r_0/2)^3} \right)$$

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

$$\underline{\underline{u}} = \varphi_0 Q + \frac{1}{3} (\varphi Q_{\pm\pm} + \varphi Q_{22} - 2\varphi Q_{33})$$

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

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



(1)

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

b) In the principal-axis system of the spheroid the quadrupole moment 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 :

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

$$\begin{aligned} \rightarrow Q_{33} &= D_{31} Q'_{11} D_{31} + D_{32} Q'_{22} D_{32} + D_{33} Q'_{33} D_{33} \\ &= q (D_{31})^2 + q (D_{32})^2 - 2q (D_{33})^2 \\ &= q [(D_{31})^2 + (D_{32})^2 - 2(D_{33})^2] \end{aligned}$$

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

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

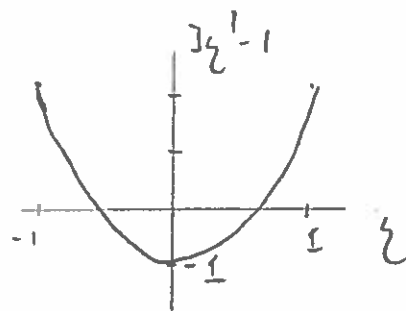
$$\rightarrow Q_{33} = q [1 - D_{33}^2 - 2D_{33}^2] = q [1 - 3\cos^2 \alpha]$$

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

$$\rightarrow \underline{u} = \varphi_0 Q - \frac{2e}{r_0^5} (A^2 - A^1) q (1 - 3\cos^2 \alpha)$$

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

c) $\int \zeta^2 - 1$ is minimized for $\zeta = 0$
 $\Leftrightarrow \mathcal{J} = \pi/2$



maximized for $\zeta = \pm 1$
 $\Leftrightarrow \mathcal{J} = 0, \pi$

let $eQ > 0$ \rightarrow u is minimized for

$$\mathcal{J} = \frac{\pi}{2} \quad \text{if } (A^2 - Q^1)(c^2 - b^2) > 0$$

$$\mathcal{J} = 0 \quad \text{if } (A^2 - Q^1)(c^2 - b^2) < 0$$

prolate spheroid ($a > b$):
 (major)



oblate ($a < b$): flips the two cones
 (disc)

$eQ < 0$: Flips the two cones again.

27.) d) 2 § 2.5, 2.5c \rightarrow The force on a single charge is $\vec{\nabla} e \varphi(\vec{x})$

\rightarrow The force on $\rho(\vec{x}) = \sum_k e_k \delta(\vec{x} - \vec{x}_k)$ is

$$\vec{F}_{el} = - \sum_k e_k \vec{\nabla} \varphi(\vec{x}) = - \int d\vec{x} \rho(\vec{x}) \vec{\nabla} \varphi(\vec{x}) \stackrel{2.5c}{=} + \int d\vec{x} \rho(\vec{x}) \vec{E}(\vec{x})$$

Now expand as in d) § 2.6:

$$\begin{aligned} F_{el}^i &= - \int d\vec{x} \rho(\vec{x}) \left[\partial_i \varphi \Big|_{\vec{x}=0} + x_j \partial_j \partial_i \varphi \Big|_{\vec{x}=0} + \dots \right] \\ &= -Q \partial_i \varphi - (\partial_i \partial_j \varphi) \Big|_{\vec{x}=0} \int d\vec{x} x_j \rho(\vec{x}) + \dots \quad \underline{Q = \int d\vec{x} \rho(\vec{x})} \\ \partial_j \varphi &= E_j \\ &= -Q \partial_i \varphi \Big|_{\vec{x}=0} + (\partial_i E_j) \Big|_{\vec{x}=0} d_j + \dots \quad \underline{\vec{d} = \int d\vec{x} \vec{x} \rho(\vec{x})} \\ &= - \partial_i \Big|_{\vec{x}=0} \left[Q \varphi - \vec{E} \cdot \vec{d} + \dots \right] \end{aligned}$$

$\rightarrow \underline{\underline{\vec{F}_{el}}} = - (\vec{\nabla} U) \Big|_{\vec{x}=0}$ with $U(\vec{x}) = Q \varphi(\vec{x}) - \vec{d} \cdot \vec{E}(\vec{x})$ for d) § 2.6
 and \vec{x} is put to zero after calculating the gradient.

In particular, the dipole term in the electrostatic energy,

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

correctly describes the potential energy of a fixed electric dipole \vec{d} in an electric field \vec{E} .