Physics 623 Homework 1

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2.3.1. **Quadrupole moments**

c) We consider a homogenously charged ellipsoid, $(x/a)^2 + (y/b)^2 + (z/c)^2 \leq 1$, and compute the quadrupole moments, Q_{2m}, where

$$Q_{lm} = \sqrt{\frac{4\pi}{2l+1}} \int_0^\infty dr\ r^2 r^l \int d\Omega \rho(r,\Omega) Y_l^m(\Omega)^* \tag{1}$$

Since the ellipsoid is homogenously charged,

$$\rho(x,y,z) = \begin{cases} \rho_0,\ (x/a)^2 + (y/b)^2 + (z/c)^2 \leq 1 \\ 0,\ \text{otherwise} \end{cases} \tag{2}$$

The spherical harmonics are given by

$$\begin{aligned} Y_2^{-2}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{-2i\phi} \sin^2(\theta) \\ Y_2^{-1}(\theta,\phi) &= \frac{1}{2}\sqrt{\frac{15}{2\pi}} e^{-i\phi} \sin(\theta)\cos(\theta) \\ Y_2^{0}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{5}{\pi}} \left(3\cos^2(\theta) - 1\right) \\ Y_2^{1}(\theta,\phi) &= -\frac{1}{2}\sqrt{\frac{15}{2\pi}} e^{i\phi} \sin(\theta)\cos(\theta) \\ Y_2^{2}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{15}{2\pi}} e^{2i\phi} \sin^2(\theta) \end{aligned} \tag{3}$$

And Q_{lm} are thus given by

$$\begin{aligned} Q_{2,-2} &= \frac{1}{2}\sqrt{\frac{3}{2}} \int_0^\infty \int dr d\Omega\ r^4 \rho(r,\Omega) e^{2i\phi} \sin^2(\theta) \\ Q_{2,-1} &= \sqrt{\frac{3}{2}} \int_0^\infty \int dr d\Omega\ r^4 \rho(r,\Omega) e^{i\phi} \sin(\theta)\cos(\theta) \\ Q_{2,0} &= \frac{1}{2} \int_0^\infty \int dr d\Omega\ r^4 \rho(r,\Omega) \left(3\cos^2(\theta) - 1\right) \\ Q_{2,1} &= -\sqrt{\frac{3}{2}} \int_0^\infty \int dr d\Omega\ r^4 \rho(r,\Omega) e^{-i\phi} \sin(\theta)\cos(\theta) \\ Q_{2,2} = Q_{2,-2}^* &= \frac{1}{2}\sqrt{\frac{3}{2}} \int_0^\infty \int dr d\Omega\ r^4 \rho(r,\Omega) e^{-2i\phi} \sin^2(\theta) \end{aligned} \tag{4}$$

We can relate the components of the quadrupole tensor, Q_{ij}, by writing the complex exponentials in terms of $\sin(\phi)$ and $\cos(\phi)$ and then rewriting the integrals in cartesian coordinates.

$$
\begin{aligned}
Q_{2,-2} &= \frac{1}{2}\sqrt{\frac{3}{2}}\int_0^\infty \int dr d\Omega \; r^4 \rho(r,\Omega) \left(\cos^2(\phi) - \sin^2(\phi) + 2i\sin(\phi)\cos(\phi)\right)\sin^2(\theta) \\
Q_{2,-1} &= \sqrt{\frac{3}{2}}\int_0^\infty \int dr d\Omega \; r^4 \rho(r,\Omega) \left(\cos(\phi) + i\sin(\phi)\right)\sin(\theta)\cos(\theta) \\
Q_{2,0} &= \frac{1}{2}\int_0^\infty \int dr d\Omega \; r^4 \rho(r,\Omega) \left(3\cos^2(\theta) - 1\right) \\
Q_{2,1} &= -\sqrt{\frac{3}{2}}\int_0^\infty \int dr d\Omega \; r^4 \rho(r,\Omega) \left(\cos(\phi) - i\sin(\phi)\right)\sin(\theta)\cos(\theta) \\
Q_{2,2} &= \frac{1}{2}\sqrt{\frac{3}{2}}\int_0^\infty \int dr d\Omega \; r^4 \rho(r,\Omega) \left(\cos^2(\phi) - \sin^2(\phi) - 2i\sin(\phi)\cos(\phi)\right)\sin^2(\theta)
\end{aligned} \tag{5}
$$

Recall that the components of the quadrupole tensor are given by

$$Q_{ij} = \frac{1}{2}\int d\mathbf{x}\rho(\mathbf{x})\left(3x_i x_j - \delta_{i,j}\mathbf{x}^2\right) \tag{6}$$

Therefore, we have the following relations

$$
\begin{aligned}
Q_{2,-2} &= \frac{1}{2}\sqrt{\frac{3}{2}}\left(\frac{2}{3}(Q_{xx} - Q_{yy}) + \frac{4}{3}iQ_{xy}\right) \\
Q_{2,-1} &= \frac{2}{3}\sqrt{\frac{3}{2}}\left(Q_{xz} + iQ_{yz}\right) \\
Q_{2,0} &= Q_{zz} \\
Q_{2,1} &= -\frac{2}{3}\sqrt{\frac{3}{2}}\left(Q_{xz} - iQ_{yz}\right) \\
Q_{2,2} &= \frac{1}{2}\sqrt{\frac{3}{2}}\left(\frac{2}{3}(Q_{xx} - Q_{yy}) - \frac{4}{3}iQ_{xy}\right)
\end{aligned} \tag{7}
$$

We know from part c) that $Q_{ij} = 0$ for $i \neq j$. Therefore, we have

$$
\begin{aligned}
Q_{2,-2} &= \frac{1}{\sqrt{6}}(Q_{xx} - Q_{yy}) \\
Q_{2,-1} &= 0 \\
Q_{2,0} &= Q_{zz} \\
Q_{2,1} &= 0 \\
Q_{2,2} &= \frac{1}{\sqrt{6}}(Q_{xx} - Q_{yy})
\end{aligned} \tag{8}
$$

Where Q_{xx}, Q_{yy}, and Q_{zz}, which were calculated in part c), are given by

$$\begin{aligned} Q_{xx} &= \frac{2\pi abc\rho_0}{15}(2a^2 - b^2 - c^2) \\ Q_{yy} &= \frac{2\pi abc\rho_0}{15}(2b^2 - a^2 - c^2) \\ Q_{zz} &= \frac{2\pi abc\rho_0}{15}(2c^2 - a^2 - b^2) \end{aligned} \tag{9}$$

So the nonzero Q_{lm} are

$$\begin{aligned} Q_{2,2} &= \frac{\sqrt{6}\pi abc\rho_0}{15}(a^2 - b^2) \\ Q_{2,0} &= \frac{2\pi abc\rho_0}{15}(2c^2 - a^2 - b^2) \end{aligned} \tag{10}$$

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

We will work in a coordinate system in which the center of the spheroid is the origin, the angle in the diagram is the spherical polar angle, and the spheroid is tilted into the y-axis.

a) We calculate the interaction energy as in the text on page 64. The interaction energy, U, is given, to quadrupole order, by

$$U = \phi_0 Q - \mathbf{E} \cdot \mathbf{d} + \frac{1}{3}\phi^{ij} Q_{ij} \tag{11}$$

where the quantities in (11) are defined as in the text. We first calculate ϕ_0, $\mathbf{E}$, and ϕ^{ij} for the lattice of charges whose charge density is $\rho_>(\mathbf{x})$. Let the charges be located at

$$\begin{aligned} \mathbf{x}_1 &= \frac{1}{2}(B, B, A) \\ \mathbf{x}_2 &= \frac{1}{2}(-B, B, A) \\ \mathbf{x}_3 &= \frac{1}{2}(-B, -B, A) \\ \mathbf{x}_4 &= \frac{1}{2}(B, -B, A) \\ \mathbf{x}_5 &= \frac{1}{2}(B, B, -A) \\ \mathbf{x}_6 &= \frac{1}{2}(-B, B, -A) \\ \mathbf{x}_7 &= \frac{1}{2}(-B, -B, -A) \\ \mathbf{x}_8 &= \frac{1}{2}(B, -B, -A) \end{aligned} \tag{12}$$

Then the potential, $\phi_>(\mathbf{x})$, is given by

$$\begin{aligned} \phi_>(\mathbf{x}) = &\frac{e}{|\mathbf{x} - \mathbf{x}_1|} + \frac{e}{|\mathbf{x} - \mathbf{x}_2|} + \frac{e}{|\mathbf{x} - \mathbf{x}_3|} + \frac{e}{|\mathbf{x} - \mathbf{x}_4|} \\ &+ \frac{e}{|\mathbf{x} - \mathbf{x}_5|} + \frac{e}{|\mathbf{x} - \mathbf{x}_6|} + \frac{e}{|\mathbf{x} - \mathbf{x}_7|} + \frac{e}{|\mathbf{x} - \mathbf{x}_8|} \end{aligned} \tag{13}$$

So we have

$$
\begin{aligned}
\phi_0 &= \phi_>(\mathbf{x}=\mathbf{0}) \\
\mathbf{E} &= -\nabla\phi_>(\mathbf{x}=\mathbf{0}) \\
\phi_{ij} &= \frac{\partial^2}{\partial x^i \partial x^j}\phi_>(\mathbf{x}=\mathbf{0}) \\
\implies \phi_0 &= \frac{8e}{\sqrt{\frac{A^2}{4}+\frac{B^2}{2}}} \\
\mathbf{E} &= \mathbf{0} \\
\phi_{xx} &= \frac{64e(A^2-B^2)}{(A^2+2B^2)^{5/2}} \\
\phi_{yy} &= \frac{64e(A^2-B^2)}{(A^2+2B^2)^{5/2}} \\
\phi_{zz} &= \frac{128e(A^2-B^2)}{(A^2+2B^2)^{5/2}} \\
\phi_{ij} &= 0, \text{ for } i \neq j
\end{aligned}
\tag{14}
$$

Therefore, the interaction energy, to quadrupole order, is

$$
U = \frac{8Qe}{\sqrt{\frac{A^2}{4}+\frac{B^2}{2}}} + \frac{1}{3}\left(\frac{64Q_{xx}e(A^2-B^2)}{(A^2+2B^2)^{5/2}} + \frac{64Q_{yy}e(A^2-B^2)}{(A^2+2B^2)^{5/2}} + \frac{128Q_{zz}e(A^2-B^2)}{(A^2+2B^2)^{5/2}}\right) \tag{15}
$$

Since Q_{ij} is traceless, $Q_{xx} = -Q_{yy} - Q_{zz}$. So we can rewrite (15) as

$$
\begin{aligned}
U &= \frac{8Qe}{\sqrt{\frac{A^2}{4}+\frac{B^2}{2}}} + \frac{1}{3}\left(-\frac{64Q_{yy}e(A^2-B^2)}{(A^2+2B^2)^{5/2}} - \frac{64Q_{zz}e(A^2-B^2)}{(A^2+2B^2)^{5/2}}\right) \\
&+ \frac{1}{3}\left(\frac{64Q_{yy}e(A^2-B^2)}{(A^2+2B^2)^{5/2}} + \frac{128Q_{zz}e(A^2-B^2)}{(A^2+2B^2)^{5/2}}\right) \\
U &= \frac{16Qe}{\sqrt{A^2+2B^2}} + \frac{64Q_{zz}e(A^2-B^2)}{3(A^2+2B^2)^{5/2}}
\end{aligned}
\tag{16}
$$

b) The quadrupole tensor of an ellipsoid, $(x/a)^2+(y/b)^2+(z/c)^2 \leq 1$, in its principle axes coordinate system was calculated in problem set 8 and was found to be

$$
Q_{ij} = \frac{1}{10}Q\begin{pmatrix} 2a^2-b^2-c^2 & 0 & 0 \\ 0 & 2b^2-a^2-c^2 & 0 \\ 0 & 0 & 2c^2-a^2-b^2 \end{pmatrix} \tag{17}
$$

In this system, we set $a \to b$, $b \to b$, and $c \to a$ to get

$$
Q'_{ij} = \frac{Q}{10}\left(b^2-a^2\right)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \tag{18}
$$

We can apply a coordinate transformation that rotates (from the principle axis system) the z-axis around the x-axis into the $-y$-axis by θ in order to transform (18) into the coordinate system of the lattice. This yields Q_{ij} by

$$\begin{aligned} Q_{ij} &= \frac{Q}{10}\left(b^2-a^2\right)\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & -\sin(\theta) \\ 0 & \sin(\theta) & \cos(\theta) \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & \sin(\theta) \\ 0 & -\sin(\theta) & \cos(\theta) \end{pmatrix} \\ Q_{ij} &= \frac{Q}{10}\left(b^2-a^2\right)\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta)^2-2\sin(\theta)^2 & 3\cos(\theta)\sin(\theta) \\ 0 & 3\cos(\theta)\sin(\theta) & \sin(\theta)^2-2\cos(\theta)^2 \end{pmatrix} \end{aligned} \tag{19}$$

Finally, we may write U as a function of θ as

$$U = \frac{16Qe}{\sqrt{A^2+2B^2}} + \frac{32Qe\left(b^2-a^2\right)\left(A^2-B^2\right)\left(\sin(\theta)^2-2\cos(\theta)^2\right)}{15(A^2+2B^2)^{5/2}} \tag{20}$$

c) The interaction energy above has equilibria when

$$\frac{\mathrm{d}U}{\mathrm{d}\theta} = \frac{32Qe\left(b^2-a^2\right)\left(A^2-B^2\right)}{15(A^2+2B^2)^{5/2}}3\sin(2\theta) = 0 \tag{21}$$

which occurs at $\theta = 0$ and $\theta = \pi/2$ (we will not distinguish between $\theta = 0$ and $\theta = \pi$). U is minimized and maximized when

$$\begin{aligned} &\frac{\mathrm{d}^2U}{\mathrm{d}\theta^2} = \frac{32Qe\left(b^2-a^2\right)\left(A^2-B^2\right)}{15(A^2+2B^2)^{5/2}}6\cos(2\theta) > 0 \\ &\text{and} \\ &\frac{\mathrm{d}^2U}{\mathrm{d}\theta^2} = \frac{32Qe\left(b^2-a^2\right)\left(A^2-B^2\right)}{15(A^2+2B^2)^{5/2}}6\cos(2\theta) < 0 \end{aligned} \tag{22}$$

respectively.
If $A > B$ and $a > b$ (prolate) then U is minimized when $\theta = \pi/2$ and maximized when $\theta = 0$.
If $A > B$ and $a < b$ (oblate) then U is minimized when $\theta = 0$ and maximized when $\theta = \pi/2$.
If $A < B$ and $a > b$ then U is minimized when $\theta = 0$ and maximized when $\theta = \pi/2$.
If $A < B$ and $a < b$ then U is minimized when $\theta = \pi/2$ and maximized when $\theta = 0$.

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

We consider a static charge distribution, $\rho(\mathbf{x})$, subject to a static potential, $\varphi(\mathbf{x})$. We claim that the force, $\mathbf{F}_{\text{el}}$, on the charge distribution obeys $\mathbf{F}_{\text{el}} = -\nabla U$, where U is the electrostatic interaction energy.

$$\mathbf{F}_{\text{el}} = \int d\mathbf{x}\ \rho(\mathbf{x})\mathbf{E}(\mathbf{x}) \tag{23}$$

We can expand $\mathbf{E}(\mathbf{x})$ to dipole order around $\mathbf{y}$ to get

$$\mathbf{F}_{\text{el}}(\mathbf{y}) = \int d\mathbf{x}\ \rho(\mathbf{x})\left(\mathbf{E}(\mathbf{y}) + \nabla_{\mathbf{y}}\mathbf{E}(\mathbf{y})(\mathbf{x}-\mathbf{y})\right) \tag{24}$$

where $\nabla_{\mathbf{y}}\mathbf{E}(\mathbf{y})$ is the field gradient tensor (acting on the vector $(\mathbf{x}-\mathbf{y})$). We can rewrite $\mathbf{E}(\mathbf{y})$ as $-\nabla_{\mathbf{y}}\varphi(\mathbf{y})$, and exchange the integral with the gradients to get

$$\begin{aligned}
\mathbf{F}_{\text{el}}(\mathbf{y}) &= \int d\mathbf{x}\ \rho(\mathbf{x})\mathbf{E}(\mathbf{y}) + \int d\mathbf{x}\ \rho(\mathbf{x})\nabla_{\mathbf{y}}\mathbf{E}(\mathbf{y})(\mathbf{x}-\mathbf{y}) \\
\mathbf{F}_{\text{el}}(\mathbf{y}) &= -\int d\mathbf{x}\ \rho(\mathbf{x})\nabla_{\mathbf{y}}\varphi(\mathbf{y}) + \int d\mathbf{x}\ \rho(\mathbf{x})\nabla_{\mathbf{y}}\mathbf{E}(\mathbf{y})(\mathbf{x}-\mathbf{y}) \\
\mathbf{F}_{\text{el}}(\mathbf{y}) &= -\nabla_{\mathbf{y}}\left(\varphi(\mathbf{y})\int d\mathbf{x}\ \rho(\mathbf{x}) - \mathbf{E}(\mathbf{y})\cdot\int d\mathbf{x}\ \rho(\mathbf{x})(\mathbf{x}-\mathbf{y})\right) \\
\mathbf{F}_{\text{el}}(\mathbf{y}) &= -\nabla_{\mathbf{y}}\left(\varphi(\mathbf{y})Q - \mathbf{E}(\mathbf{y})\cdot\mathbf{d} + \mathbf{E}(\mathbf{y})\cdot\mathbf{y}Q\right)
\end{aligned} \tag{25}$$

Now, evaluating (25) at $\mathbf{y}=\mathbf{0}$, we have

$$\begin{aligned}
\mathbf{F}_{\text{el}}(\mathbf{y})\Big|_{\mathbf{y}=\mathbf{0}} &= -\nabla_{\mathbf{y}}\left(\varphi(\mathbf{y})Q - \mathbf{E}(\mathbf{y})\cdot\mathbf{d}\right)\Big|_{\mathbf{y}=\mathbf{0}} \\
\mathbf{F}_{\text{el}}(\mathbf{y})\Big|_{\mathbf{y}=\mathbf{0}} &= -\nabla_{\mathbf{y}}U\Big|_{\mathbf{y}=\mathbf{0}} \\
\implies \mathbf{F}_{\text{el}} &= -\nabla U
\end{aligned} \tag{26}$$

In particular, supposing $Q=0$, then we have $\mathbf{F}_{\text{el}} = \nabla\left(\mathbf{E}\cdot\mathbf{d}\right)$, as expected.

♣