Problem 4.7

A localized distribution of charge has a charge density

$$\rho(\mathbf{r}) = \frac{1}{64\pi} r^2 e^{-r} \sin^2\theta$$

(a) Make a multipole expansion of the potential due to this charge density and determine all the nonvanishing multipole moments. Write down the potential at large distances as a finite expansion in Legendre polynomials.

(b) Determine the potential explicitly at any point in space, and show that near the origin, correct to r^2 inclusive,

$$\Phi(\mathbf{r}) \simeq \frac{1}{4\pi\epsilon_0}\left[\frac{1}{4} - \frac{r^2}{120}P_2(\cos\theta)\right].$$

(c) If there exists at the origin a nucleus with a quadrupole moment $Q = 10^{-28}\text{m}^2$, determine the magnitude of the interaction energy, assuming that the unit of charge in $\rho(\mathbf{r})$ above is the electronic charge and the unit of length is the hydrogen Bohr radius $a_0 = 4\pi\epsilon_0\hbar^2/me^2 = 0.529 \times 10^{-10}\text{m}$. Express your answer as a frequency by dividing by Planck's constant h. The charge density in this problem is that for the $m = \pm 1$ states of the $2p$ level in hydrogen, while the quadrupole interaction is of the same order as found in molecules.

Solution.

(a) Note that the charge density is not localized. However, since it decays exponentially we can safely perform a multipole expansion very far away (see the footnote in p.145). The potential is given by

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\mathrm{d}^3x' = \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}q_{lm}\frac{Y_{lm}(\theta,\phi)}{r^{l+1}},$$

where

$$q_{lm} = \int Y_{lm}^*(\theta',\phi')r'^l\rho(\mathbf{x}')\mathrm{d}^3x'.$$

Due to the azimuthal symmetry of the charge density only the q_{l0} terms can be nonzero. Using Equation 3.57 for $Y_{l0} = Y_{l0}^*$, the nonvanishing multipole moments are

$$\begin{aligned}
q_{l0} &= \sqrt{\frac{2l+1}{4\pi}}\int P_l(\cos\theta')r'^l\rho(\mathbf{x}')\mathrm{d}^3x' \\
&= \sqrt{\frac{2l+1}{4\pi}}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} P_l(\cos\theta')r'^l\rho(\mathbf{x}')r'^2\sin\theta'\mathrm{d}r'\mathrm{d}\theta'\mathrm{d}\phi' \\
&= \sqrt{(2l+1)\pi}\int_0^{\pi}\int_0^{\infty} P_l(\cos\theta')r'^{l+2}\rho(\mathbf{x}')\sin\theta'\mathrm{d}r'\mathrm{d}\theta' \\
&= \frac{1}{64}\sqrt{\frac{2l+1}{\pi}}\int_0^{\infty} r'^{l+4}e^{-r'}\mathrm{d}r'\int_0^{\pi} P_l(\cos\theta')\sin^3\theta\mathrm{d}\theta' \\
&= \frac{1}{64}\sqrt{\frac{2l+1}{\pi}}\Gamma(l+5)\int_0^{\pi} P_l(\cos\theta')\sin^3\theta'\mathrm{d}\theta'.
\end{aligned}$$

Note that $\sin^3\theta$ is symmetric (even) about $\pi/2$. Now, $P_l(\cos\theta)$ is also symmetric about $\pi/2$ for even l, while it is antisymmetric (odd) for odd l. Thus, only even l's can be nonzero. (This can also be deduced by noting that the charge density is plane symmetric about $z = 0$.)

$$\begin{aligned} q_{2l,0} &= \frac{1}{64}\sqrt{\frac{4l+1}{\pi}}\Gamma(2l+5)\int_0^\pi P_{2l}(\cos\theta')\sin^3\theta' \mathrm{d}\theta' \\ &= \frac{1}{64}\sqrt{\frac{4l+1}{\pi}}\Gamma(2l+5)\int_{-1}^1 P_{2l}(\cos\theta')\sin^2\theta' \mathrm{d}(\cos\theta') \end{aligned}$$

Now, observe that

$$\sin^2\theta' = 1-\cos^2\theta' = -\frac{1}{3}(3\cos^2\theta'-1)+\frac{2}{3} = \frac{2}{3}\left(P_0(\cos\theta')-P_2(\cos\theta')\right).$$

Therefore only the monopole and quadrupole moments are nonzero by the orthogonality of the Legendre polynomials. Thus, using Equation 3.21

$$\begin{aligned} q_{00} &= \frac{1}{64}\sqrt{\frac{1}{\pi}}\Gamma(5)\cdot\frac{2}{3}\cdot 2 = \frac{1}{48}\frac{1}{\sqrt{\pi}}\Gamma(5) = \frac{1}{2\sqrt{\pi}}, \\ q_{20} &= \frac{1}{64}\sqrt{\frac{5}{\pi}}\Gamma(7)\cdot\left(-\frac{2}{3}\right)\cdot\frac{2}{5} = -\frac{1}{240}\sqrt{\frac{5}{\pi}}\Gamma(7) = -3\sqrt{\frac{5}{\pi}}. \end{aligned}$$

Thus, the potential at large distances is

$$\begin{aligned} \Phi(\mathbf{x}) &= \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{1}\frac{4\pi}{4l+1}q_{2l,0}\frac{Y_{2l,0}(\theta,\phi)}{r^{2l+1}} \\ &= \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{1}\sqrt{\frac{4\pi}{4l+1}}q_{2l,0}\frac{P_{2l}(\cos\theta)}{r^{2l+1}} \\ &= \frac{1}{4\pi\epsilon_0}\sqrt{4\pi}\,q_{00}\frac{P_0(\cos\theta)}{r} + \frac{1}{4\pi\epsilon_0}\sqrt{\frac{4\pi}{5}}q_{20}\frac{P_2(\cos\theta)}{r^3} \\ &= \frac{1}{4\pi\epsilon_0}\frac{1}{r} - \frac{3}{2\pi\epsilon_0}\frac{P_2(\cos\theta)}{r^3}. \end{aligned}$$

(b) Near the origin, we can no longer blindly use the multipole expansion. Therefore, we must start from Coulomb's law. Note that we can first solve for the potential at the z axis, and then add the Legendre polynomial correction later. Again, since there is azimuthal symmetry we can expand $1/|\mathbf{x}-\mathbf{x}'|$ in terms of Legendre polynomials. We obtain

$$\begin{aligned} \Phi(z) &= \frac{1}{4\pi\epsilon_0}\int\frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\mathrm{d}^3x' \\ &= \frac{1}{4\pi\epsilon_0}\int_0^{2\pi}\int_0^\pi\int_0^\infty\left(\frac{1}{64\pi}r'^2e^{-r'}\sin^2\theta'\right)\sum_{l=0}^\infty\frac{r_<^l}{r_>^{l+1}}P_l(\cos\theta')r'^2\sin\theta'\mathrm{d}r'\mathrm{d}\theta'\mathrm{d}\phi' \\ &= \frac{1}{128\pi\epsilon_0}\sum_{l=0}^\infty\int_0^\infty r'^4\frac{r_<^l}{r_>^{l+1}}e^{-r'}\mathrm{d}r'\int_0^\pi P_l(\cos\theta')\sin^3\theta'\mathrm{d}\theta'. \end{aligned}$$

We already know that the second integral is only nonzero when $l = 0$ or $l = 2$. Therefore,

$$\begin{aligned}\Phi(z)\Big|_z &= \Phi(z)_{l=0} + \Phi(z)_{l=2} \\ &= \frac{1}{128\pi\epsilon_0}\left(\frac{4}{3}\int_0^\infty \frac{r'^4}{r_>}e^{-r'}\mathrm{d}r' - \frac{4}{15}\int_0^\infty r'^4\frac{r_<^2}{r_>^3}e^{-r'}\mathrm{d}r'\right).\end{aligned}$$

Suppose we want to find the potential at $z = r$. Then we must split the integral. For if $r' < r$ then clearly $r_< = r'$ and $r_> = r$; conversely for $r' > r$. Therefore,

$$\begin{aligned}\Phi(z = r) = {} & \frac{1}{96\pi\epsilon_0}\left(\int_0^r \frac{r'^4}{r}e^{-r'}\mathrm{d}r' + \int_r^\infty r'^3 e^{-r'}\mathrm{d}r'\right) \\ & - \frac{1}{480\pi\epsilon_0}\left(\int_0^r \frac{r'^6}{r^3}e^{-r'}\mathrm{d}r' + \int_r^\infty r^2 r' e^{-r'}\mathrm{d}r'\right)\end{aligned}$$

In the general case where $\mathbf{x}$ is not in the z axis, the potential is simply

$$\begin{aligned}\Phi(\mathbf{x}) = {} & \frac{1}{96\pi\epsilon_0}\left(\int_0^r \frac{r'^4}{r}e^{-r'}\mathrm{d}r' + \int_r^\infty r'^3 e^{-r'}\mathrm{d}r'\right) \\ & - \frac{1}{480\pi\epsilon_0}\left(\int_0^r \frac{r'^6}{r^3}e^{-r'}\mathrm{d}r' + \int_r^\infty r^2 r' e^{-r'}\mathrm{d}r'\right) P_2(\cos\theta).\end{aligned}$$

Explicitly, we get the ugly expression

$$\begin{aligned}\Phi(\mathbf{x}) = {} & \frac{1}{96\pi\epsilon_0}\left[\frac{24}{r}(1 - e^{-r}) - e^{-r}(18 + r(r+6))\right] \\ & - \frac{1}{480\pi\epsilon_0}\left[\frac{720}{r^3} - \frac{5}{r^3}e^{-r}\left(144 + r(r^2+12)(r^2+6r+12)\right)\right] P_2(\cos\theta).\end{aligned}$$

Since e^{-r} decays faster than any power, we see that very far away the potential reduces to

$$\begin{aligned}\Phi(\mathbf{x}) &\simeq \frac{1}{96\pi\epsilon_0}\left(\frac{24}{r}\right) - \frac{1}{480\pi\epsilon_0}\left(\frac{720}{r^3}\right) P_2(\cos\theta) \\ &\simeq \frac{1}{4\pi\epsilon_0}\frac{1}{r} - \frac{3}{2\pi\epsilon_0}\frac{P_2(\cos\theta)}{r^3},\end{aligned}$$

as expected. Now, near the origin we can safely assume that $r_< = r$ and $r_> = r'$ always; so that we may ignore the integral from zero to r, and the other integral may be taken from zero to infinity. Thus,

$$\begin{aligned}\Phi(\mathbf{x}) &\simeq \frac{1}{96\pi\epsilon_0}\int_0^\infty r'^3 e^{-r'}\mathrm{d}r' - \frac{1}{480\pi\epsilon_0}\int_0^\infty r^2 r' e^{-r'}\mathrm{d}r' \cdot P_2(\cos\theta) \\ &\simeq \frac{1}{96\pi\epsilon_0}\Gamma(4) - \frac{r^2}{480\pi\epsilon_0}\Gamma(2)\cdot P_2(\cos\theta) \\ &\simeq \frac{1}{4\pi\epsilon_0}\left[\frac{1}{4} - \frac{r^2}{120}P_2(\cos\theta)\right].\end{aligned}$$

Alternatively, we can expand the exact expression as a power series in r around the origin. We will find that the first bracket is $6 + \mathcal{O}(r^3)$ and the second bracket is $r^2 + \mathcal{O}(r^3)$.

(c) The interaction energy is given by

$$\begin{aligned}
W &= \int \rho(\mathbf{x})\Phi(\mathbf{x})\mathrm{d}^3x \\
&\simeq \int \rho \left[\frac{1}{4\pi\epsilon_0}\left(\frac{1}{4} - \frac{r^2}{120}P_2(\cos\theta)\right)\right]\mathrm{d}^3x \\
&\simeq \int \rho \left[\frac{-e^2}{4\pi\epsilon_0 a_0}\left(\frac{1}{4} - \frac{1}{120}\left(\frac{r^2}{a_0^2}\right)P_2(\cos\theta)\right)\right]\mathrm{d}^3x \\
&\simeq \frac{e^2}{480\pi\epsilon_0 a_0^3}\int \rho r^2 P_2(\cos\theta)\mathrm{d}^3x \\
&\simeq \frac{e^2}{480\pi\epsilon_0 a_0^3}\frac{1}{2}\int \rho r^2(3\cos^2\theta - 1)\mathrm{d}^3x \\
&\simeq \frac{e^2}{960\pi\epsilon_0 a_0^3}\int \rho(3z^2 - r^2)\mathrm{d}^3x \\
&\simeq \frac{Qe^2}{960\pi\epsilon_0 a_0^3} \\
\frac{W}{h} &\simeq 1\text{MHz}.
\end{aligned}$$

$\square$