Jackson 4.7 Homework Problem Solution

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PROBLEM:

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 non-vanishing 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 the solution near the origin, correct to r^2 inclusive,

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

(c) If there exists at the origin a nucleus with a quadrupole moment $Q = 10^{-28}$ 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 $a_0 = 4\pi\epsilon_0 \hbar^2 / m e^2 = 0.529\times10^{-10} m$. Express your answer as a frequency by dividing by Plank's constant h.

The charge density in this problem is that for the $m=\pm1$ states of the 2p level in hydrogen, while the quadrupole interaction is of the same order as found in molecules.

SOLUTION:

(a) The general solution in terms of a multipole expansion of a localized distribution in spherical harmonics is:

$$\Phi(r,\theta,\phi) = \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1} q_{lm}\frac{Y_{lm}(\theta,\phi)}{r^{l+1}} \quad \text{where} \quad q_{lm} = \int Y^*_{lm}(\theta',\phi') r'^l \rho(\mathbf{x}') d\mathbf{x}'$$

For cases where there is azimuthal symmetry in the charge distribution, this reduces to:

$$\Phi(r,\theta,\phi) = \frac{1}{4\pi\epsilon_0}\sum_{l=0}^{\infty}\sqrt{\frac{4\pi}{2l+1}} q_l \frac{P_l(\cos\theta)}{r^{l+1}} \quad \text{where}$$

$$q_l = 2\pi\sqrt{\frac{2l+1}{4\pi}}\int_0^{\pi}\int_0^{\infty} P_l(\cos\theta') r'^{l+2}\rho(r',\theta')\sin\theta' dr' d\theta'$$

Let us now plug in the charge density for this case:

$$q_l = \frac{1}{64\pi} 2\pi \sqrt{\frac{2l+1}{4\pi}} \int_{-1}^{1} P_l(x')(1-x'^2)\, dx' \int_0^\infty r'^{l+4} e^{-r'}\, dr'$$

Use the identity easily found in an integral table: $\int_0^\infty x^n e^{-x}\, dx = n!$ if n is a positive integer, which is the case here.

$$q_l = \frac{1}{64\pi} 2\pi \sqrt{\frac{2l+1}{4\pi}} (l+4)! \int_{-1}^{1} P_l(x')(1-x'^2)\, dx'$$

We can use the identity: $x'^2 = \frac{2}{3} P_2(x') + \frac{1}{3} P_0(x')$ which is easily derived from the definition of the two specific Legendre polynomials.

$$q_l = \frac{1}{64\pi} 2\pi \sqrt{\frac{2l+1}{4\pi}} (l+4)! \left[-\frac{2}{3} \int_{-1}^{1} P_l(x') P_2(x')\, dx' + \frac{2}{3} \int_{-1}^{1} P_l(x') P_0(x')\, dx' \right]$$

Due to orthogonality, every q_l is zero except when $l = 0$ or $l = 2$:

$$q_0 = \sqrt{\frac{1}{4\pi}}$$

$$q_2 = -3\sqrt{\frac{5}{\pi}}$$

We can now find the final solution to the potential:

$$\Phi(r,\theta,\phi) = \frac{1}{4\pi\epsilon_0} \left[\sqrt{4\pi}\, q_0 \frac{1}{r} + \sqrt{\frac{\pi}{5}}\, q_2 \frac{3\cos^2\theta - 1}{r^3} \right]$$

$$\boxed{\Phi(r,\theta,\phi) = \frac{1}{4\pi\epsilon_0} \left[\frac{1}{r} + \frac{3 - 9\cos^2\theta}{r^3} \right]}$$

or in terms of Legendre polynomials:

$$\boxed{\Phi(r,\theta,\phi) = \frac{1}{4\pi\epsilon_0} \left[\frac{P_0(\cos\theta)}{r} - 6\frac{P_2(\cos\theta)}{r^3} \right]}$$

Note that this solution is exact as long as the observation point is beyond the edge of the charge density. There is no "far-away" limitation to this solution because all higher order terms are zero. Unfortunately, in this problem, there is no clearly defined "edge" to the charge density. This solution becomes exact once e^{-r} is so small so as to be negligible.

(b) The multipole expansion is only valid if the observation point is external to a local charge distribution. To find the potential within the charge distribution, we must use Coulomb's law:

$$\Phi=\frac{1}{4\pi\epsilon_0}\int\frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}d\,\mathbf{x}'$$

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{64\pi}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\frac{r'^2e^{-r'}\sin^2\theta'}{|\mathbf{x}-\mathbf{x}'|}r'^2\sin\theta'\,dr'\,d\theta'\,d\phi'$$

Expand the denominator in spherical harmonics

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{64\pi}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}r'^4e^{-r'}\sin^2\theta'\,4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{1}{2l+1}\frac{r_<^l}{r_>^{l+1}}Y_{lm}^*(\theta',\phi')Y_{lm}(\theta,\phi)\sin\theta'\,dr'\,d\theta'\,d\phi'$$

Due to azimuthal symmetry, only the $m=0$ terms will survive.

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{32}\sum_{l=0}^{\infty}P_l(\cos\theta)\int_{-1}^{1}P_l(x')(1-x'^2)\,d\,x'\int_0^{\infty}r'^4e^{-r'}\frac{r_<^l}{r_>^{l+1}}dr'$$

Again use the identity: $x'^2=\frac{2}{3}P_2(x')+\frac{1}{3}P_0(x')$

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{32}\sum_{l=0}^{\infty}P_l(\cos\theta)[-\frac{2}{3}\int_{-1}^{1}P_l(x')P_2(x')\,d\,x'+\frac{2}{3}\int_{-1}^{1}P_l(x')P_0(x')\,d\,x']\int_0^{\infty}r'^4e^{-r'}\frac{r_<^l}{r_>^{l+1}}dr'$$

Due to orthogonality, all terms drop out except $l=0$ and $l=2$:

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{32}\left[\frac{4}{3}\int_0^{\infty}r'^4e^{-r'}\frac{1}{r_>}dr'-\frac{4}{15}P_2(\cos\theta)\int_0^{\infty}r'^4e^{-r'}\frac{r_<^2}{r_>^3}dr'\right]$$

We must break each integral into two cases, when $r'<r$ and $r'>r$

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{32}[\frac{4}{3}\frac{1}{r}\int_0^{r}r'^4e^{-r'}\,dr'+\frac{4}{3}\int_r^{\infty}r'^3e^{-r'}\,dr'$$
$$-\frac{4}{15}P_2(\cos\theta)\frac{1}{r^3}\int_0^{r}r'^6e^{-r'}\,dr'-\frac{4}{15}P_2(\cos\theta)r^2\int_r^{\infty}r'e^{-r'}\,dr']$$

$$\Phi=\frac{1}{4\pi\epsilon_0}\frac{1}{32}[\frac{4}{3}\frac{1}{r}\left[e^{-r'}(-r'^4-4r'^3-12r'^2-24r'-24)\right]_0^r+\frac{4}{3}\left[e^{-r'}(-r'^3-3r'^2-6r'-6)\right]_r^{\infty}$$
$$-\frac{4}{15}P_2(\cos\theta)\left(\frac{1}{r^3}\left[e^{-r'}(-r'^6-6r'^5-30r'^4-120r'^3-360r'^2-720r'-720)\right]_0^r+r^2\left[-e^{-r'}(r'+1)\right]_r^{\infty}\right)]$$

$$\Phi=\frac{1}{4\pi\epsilon_0}[\frac{1}{24}\left[-e^{-r}(r^2+6r+18+\frac{24}{r})+\frac{24}{r}\right]$$
$$-P_2(\cos\theta)\frac{1}{120}\left[e^{-r}(-5r^2-30r-120-\frac{360}{r}-\frac{720}{r^2}-\frac{720}{r^3})+\frac{720}{r^3}\right]]$$

This solution is exact and applies everywhere.
We can take the limit as e^{-r} becomes zero to check the solution obtained using multipole moments. We find:

$$\Phi(r,\theta,\phi)=\frac{1}{4\pi\epsilon_0}\left[\frac{P_0(\cos\theta)}{r}-6\frac{P_2(\cos(\theta))}{r^3}\right]$$

This matches the far-away solution found using the multipole expansion.

We can also take the limit close to the origin. We must first expand the exponential into a Taylor series:

$$e^{-r}=1-r+\frac{1}{2}r^2-\frac{1}{6}r^3+\frac{1}{24}r^4-\frac{1}{120}r^5+...$$

After distributing out all terms, we can throw out terms r^3, r^4 and higher because they contribute very little near the origin.

$$\Phi\approx\frac{1}{4\pi\epsilon_0}[\frac{1}{24}\left[-r^2-6r-18-\frac{24}{r}+6r^2+18r+24-9r^2-12r+4r^2+\frac{24}{r}\right]$$
$$-P_2(\cos\theta)\frac{1}{120}[-5r^2-30r+30r^2-120+120r-120\frac{1}{2}r^2-\frac{360}{r}+360-180r+60r^2-\frac{720}{r^2}$$
$$+\frac{720}{r}-360+120r-30r^2-\frac{720}{r^3}+\frac{720}{r^2}-\frac{360}{r}+120-30r+6r^2+\frac{720}{r^3}]]$$

Most of these terms cancel out and the final solution close to the origin reduces to:

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

(c) We are to assume that the charge density of the previous parts, and its associated potential, is the average charge distribution of a single electron bound to a hydrogen nucleus. The nucleus of is so small that is can be considered as contained at the origin, so that we only need to use the expression for the electron's potential near the origin (the last equation of part b). If we convert from units of elementary charge and Bohr radius lengths to SI units, the potential of the electron near the origin becomes:

$$\Phi\approx\frac{-e}{4\pi\epsilon_0 a_0}\left[\frac{1}{4}-\frac{(r/a_0)^2}{120}P_2(\cos\theta)\right]$$

The interaction energy is the total potential energy between the interacting electron's potential and nucleus' charge:

$$W = \int \rho_{\text{nucl}} \Phi_{\text{elec}} d^3 x$$

$$W = \int \rho_{\text{nucl}} \frac{-e}{4\pi \epsilon_0 a_0} \left[\frac{1}{4} - \frac{(r/a_0)^2}{120} P_2(\cos\theta) \right] d^3 x$$

$$W = \frac{-e}{4\pi \epsilon_0 a_0} \left[\frac{1}{4} q_{\text{nucl}} - \frac{1}{240 a_0^2} \int \rho_{\text{nucl}} (3z^2 - r^2) d^3 x \right]$$

$$W = \frac{-e}{4\pi \epsilon_0 a_0} \left[\frac{1}{4} q_{\text{nucl}} - \frac{e}{240 a_0^2} Q_{zz,\text{nucl}} \right]$$

The problem does not explicitly ask for the monopole moment interaction of the nucleus. We drop the first term and find:

$$\frac{W}{h} = \frac{\alpha c Q_{zz,\text{nucl}}}{480 \pi a_0^3}$$ where the zero-energy fine structure constant is $\alpha = \frac{e^2}{4\pi \epsilon_0 \hbar c} \approx 7.3 \times 10^{-3}$

$$\boxed{\frac{W}{h} \approx 1\,\text{MHz}}$$