1. By definition

$$\begin{aligned} q_{lm} &= \int Y^*_{lm}(\theta,\phi)\, r^l \rho(\mathbf{x})\, d^3x \\ &= \frac{1}{64\pi}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\int_0^\infty r^{l+4}e^{-r}dr \int_0^\pi P_l^m(\cos\theta)\cdot\sin^2\theta\sin\theta d\theta\int_0^{2\pi} e^{-im\phi}d\phi \\ &= \frac{2\pi\delta_{m0}}{64\pi}\sqrt{\frac{2l+1}{4\pi}}(l+4)!\int_{-1}^1 P_l(y)\left(1-y^2\right)dy \end{aligned} \tag{1}$$

Since

$$1-y^2 = \frac{2}{3}-\frac{2}{3}\cdot\frac{1}{2}\left(3y^2-1\right) = \frac{2}{3}\left[P_0(y)-P_2(y)\right] \tag{2}$$

By orthonormality of Legendre polynomials, we have

$$q_{lm} = \begin{cases} \frac{1}{2}\sqrt{\frac{1}{\pi}} & \text{for } l=0, m=0 \\ -3\sqrt{\frac{5}{\pi}} & \text{for } l=2, m=0 \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

Using equation (4.1), we have the potential at large distance:

$$\begin{aligned} \Phi(\mathbf{x}) &= \frac{1}{4\pi\epsilon_0}\left[4\pi q_{00}\frac{Y_{00}(\theta,\phi)}{r}+\frac{4\pi}{5}q_{20}\frac{Y_{20}(\theta,\phi)}{r^3}\right] \\ &= \frac{1}{4\pi\epsilon_0}\left[4\pi\cdot\frac{1}{2}\sqrt{\frac{1}{\pi}}\frac{\sqrt{\frac{1}{4\pi}}P_0(\cos\theta)}{r}+\frac{4\pi}{5}\left(-3\sqrt{\frac{5}{\pi}}\right)\frac{\sqrt{\frac{5}{4\pi}}P_2(\cos\theta)}{r^3}\right] \\ &= \frac{1}{4\pi\epsilon_0}\left[\frac{P_0(\cos\theta)}{r}-\frac{6P_2(\cos\theta)}{r^3}\right] \end{aligned} \tag{4}$$

2. For arbitrary point in space, the potential is given from the first principles:

$$\begin{aligned} \Phi(\mathbf{x}) &= \frac{1}{4\pi\epsilon_0}\int\frac{\rho(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}d^3x' && \text{(by eq 3.38)} \\ &= \frac{1}{4\pi\epsilon_0}\frac{1}{64\pi}\int r'^2e^{-r'}\sin^2\theta'\left[\sum_l\frac{r_<^l}{r_>^{l+1}}P_l(\cos\gamma)\right]d^3x' && \text{(by addition theorem)} \\ &= \frac{1}{4\pi\epsilon_0}\frac{1}{64\pi}\int r'^2e^{-r'}\sin^2\theta'\sum_{l,m}\frac{r_<^l}{r_>^{l+1}}\frac{4\pi}{2l+1}Y^*_{lm}\left(\theta',\phi'\right)Y_{lm}(\theta,\phi)\,d^3x' \end{aligned} \tag{5}$$

Now it's clear that the $d\phi'$ integral ensures only $m=0$ can contribute, so (5) is reduced to

$$\begin{aligned} \Phi(\mathbf{x}) &= \frac{1}{4\pi\epsilon_0}\frac{1}{64\pi}\cdot 2\pi\sum_l P_l(\cos\theta)\int_0^\infty r'^2e^{-r'}\frac{r_<^l}{r_>^{l+1}}r'^2dr'\cdot\underbrace{\int_0^\pi\sin^2\theta' P_l\left(\cos\theta'\right)\sin\theta' d\theta'}_{\frac{4}{3}\delta_{l0}-\frac{4}{15}\delta_{l2}\text{ by (2)}} \\ &= \frac{1}{96\pi\epsilon_0}\underbrace{\int_0^\infty r'^4e^{-r'}\frac{1}{r_>}dr'}_{A}-\frac{1}{480\pi\epsilon_0}P_2(\cos\theta)\underbrace{\int r'^4e^{-r'}\frac{r_<^2}{r_>^3}dr'}_{B} \end{aligned} \tag{6}$$

Let

$$I_k \equiv \int_0^r r'^k e^{-r'}dr' \qquad \text{and} \qquad J_k \equiv \int_r^\infty r'^k e^{-r'}dr' \tag{7}$$

we have

$$I_k = -r'^k e^{-r'}\Big|_0^r + k\int_0^r r'^{k-1}e^{-r'}dr' = -r^k e^{-r} + kI_{k-1} \qquad I_0 = 1-e^{-r} \tag{8}$$

$$J_k = -r'^k e^{-r'}\Big|_r^\infty + k\int_r^\infty r'^{k-1}e^{-r'}dr' = r^k e^{-r} + kJ_{k-1} \qquad J_0 = e^{-r} \tag{9}$$

Thus in (6)

$$\begin{aligned}
A =& \frac{1}{r}I_4 + J_3\\
=& \frac{1}{r}\left(-r^4e^{-r} + 4\left(-r^3e^{-r} + 3\left(-r^2e^{-r} + 2\left(-re^{-r} + \left(1-e^{-r}\right)\right)\right)\right)\right)\\
&+ \left(r^3e^{-r} + 3\left(r^2e^{-r} + 2\left(re^{-r} + e^{-r}\right)\right)\right)\\
=& -r^2e^{-r} - 6re^{-r} - 18e^{-r} + \frac{24}{r} - 24\frac{e^{-r}}{r}\\
=& -r^2\cdot 1 - 6r(1-r) - 18\left(1-r+\frac{r^2}{2}\right) + \frac{24}{r} - 24\cdot\frac{1-r+\frac{r^2}{2}-\frac{r^3}{6}}{r} + O\left(r^3\right)\\
=& 6 + O\left(r^3\right)
\end{aligned} \tag{10}$$

$$\begin{aligned}
B =& \frac{1}{r^3}I_6 + r^2J_1\\
=& \frac{1}{r^3}\Big[-r^6e^{-r} - 6r^5e^{-r} - 6\cdot 5r^4e^{-r} - 6\cdot 5\cdot 4r^3e^{-r}\\
&\quad - 6\cdot 5\cdot 4\cdot 3r^2e^{-r} - 6\cdot 5\cdot 4\cdot 3\cdot 2re^{-r} + 6\cdot 5\cdot 4\cdot 3\cdot 2\cdot 1\left(1-e^{-r}\right)\Big]\\
&+ r^2\left(re^{-r} + e^{-r}\right)\\
=& -5r^2e^{-r} - 30re^{-r} - 120e^{-r} - 360\frac{e^{-r}}{r} - 720\frac{e^{-r}}{r^2} + \frac{720}{r^3} - 720\frac{e^{-r}}{r^3}\\
=& -5r^2 - 30r(1-r) - 120\left(1-r+\frac{r^2}{2}\right)\\
&- 360\cdot\frac{1-r+\frac{r^2}{2}-\frac{r^3}{6}}{r} - 720\cdot\frac{1-r+\frac{r^2}{2}-\frac{r^3}{6}+\frac{r^4}{24}}{r^2} + \frac{720}{r^3}\\
&- 720\cdot\frac{1-r+\frac{r^2}{2}-\frac{r^3}{6}+\frac{r^4}{24}-\frac{r^5}{120}}{r^3} + O\left(r^3\right)\\
=& r^2 + O\left(r^3\right)
\end{aligned} \tag{11}$$

Inserting (10) and (11) back to (6) gives us up to r^2 order,

$$\Phi(\mathbf{x}) \approx \frac{1}{4\pi\epsilon_0}\left[\frac{1}{4} - \frac{r^2}{120}P_2(\cos\theta)\right] \tag{12}$$

3. For this part, we can calculate in two ways. But before that, let's first rewrite (12) with the right dimension:

$$\Phi(\mathbf{x}) = \frac{e}{4\pi\epsilon_0 a_0}\left[\frac{1}{4} - \frac{1}{120}\left(\frac{r}{a_0}\right)^2 P_2(\cos\theta)\right] \tag{13}$$

(a) Let $\eta(\mathbf{x})$ be the charge density of the nucleus, then the energy of the nucleus in the external field (13) is

$$\begin{aligned}
W =& \int \eta(\mathbf{x})\Phi(\mathbf{x})\,d^3x\\
=& \frac{e}{4\pi\epsilon_0 a_0}\left[\frac{1}{4}\int \eta(\mathbf{x})\,d^3x - \frac{1}{120a_0^2}\frac{1}{2}\int \eta(\mathbf{x})\left(3z^2-r^2\right)d^3x\right]
\end{aligned} \tag{14}$$

where we identify the first term as the energy of monopole interaction (in which we are not interested), and the second term as the energy of quadrupole interaction, which is

$$W^{(2)} = -\frac{e}{4\pi\epsilon_0 a_0} \cdot \frac{1}{240a_0^2} Q_{33} = -\frac{e^2 Q}{960\pi\epsilon_0 a_0^3} \tag{15}$$

(b) Recall in prob 4.6 (a), we have calculated the energy of quadrupole interaction as

$$W^{(2)} = -\frac{e}{4} Q \left(\frac{\partial E_z}{\partial z}\right)_0 = \frac{e}{4} Q \left(\frac{\partial^2 \Phi}{\partial z^2}\right)_0 \tag{16}$$

From (13), we know

$$\left(\frac{\partial^2 \Phi}{\partial z^2}\right)_0 = -\left\{\frac{\partial^2}{\partial z^2}\left[\frac{e}{480\pi\epsilon_0 a_0^3} \frac{1}{2}\left(3z^2 - r^2\right)\right]\right\}_0 = -\frac{e}{240\pi\epsilon_0 a_0^3} \tag{17}$$

which turns (16) into (15), agreeing with method (a).

The numerical calculation yields

$$W^{(2)}/h = -\frac{e^2 Q}{960\pi\epsilon_0 a_0^3 h} \approx 0.98\text{MHz} \tag{18}$$