1 Problem 4.1

1.1

charge	r	θ	φ
$+q$	a	$\pi/2$	0
$+q$	a	$\pi/2$	$\pi/2$
$-q$	a	$\pi/2$	π
$-q$	a	$\pi/2$	$3\pi/2$

$$\begin{aligned}
q_{l,m} =& qa^l \left[Y^*_{l,m}(\theta=\pi/2,\varphi=0) + Y^*_{l,m}(\theta=\pi/2,\varphi=\pi/2)\right.\\
&\left. - Y^*_{l,m}(\theta=\pi/2,\varphi=\pi) - Y^*_{l,m}(\theta=\pi/2,\varphi=3\pi/2)\right]\\
=& qa^l(-1)^m\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}}\left[\underbrace{e^{i(-m)(0)}}_{1} + \underbrace{e^{i(-m)(\pi/2)}}_{(-i)^m} - \underbrace{e^{i(-m)(\pi)}}_{(-1)^m} - \underbrace{e^{i(-m)(3\pi/2)}}_{i^m}\right] P_l^{-m}\left(\cancelto{0}{\cos(\pi/2)}\right)\\
=& qa^l\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}}\left[1 + (-i)^m - (-1)^m - i^m\right] P_l^{-m}(0)\\
=& qa^l\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} P_l^{-m}(0)\begin{cases}0 & m \text{ even}\\ 2-2i(-1)^{(m-1)/2} & m \text{ odd}\end{cases}
\end{aligned}$$

$l = 1$:

$$q_{1,1} = -q^*_{1,-1} = -qa\sqrt{\frac{3}{2\pi}}(1-i)$$

$l = 3$:

$$\begin{aligned}
q_{3,1} = -q^*_{3,-1} = qa^3\sqrt{\frac{7}{\pi}}(2-2i)\left(-\frac{1}{12}\right)\left(-\frac{3}{2}\right) = qa^3\sqrt{\frac{7}{\pi}}(1-i)\frac{1}{4}\\
q_{3,3} = -q^*_{3,-3} = qa^3\sqrt{\frac{1260}{\pi}}(2+2i)\left(-\frac{1}{720}\right)(-15) = qa^3\sqrt{\frac{35}{\pi}}(1+i)\frac{1}{4}
\end{aligned}$$

1.2

charge	r	θ	φ
$+q$	a	0	0
$-2q$	0	0	0
q	a	π	0

$$
\begin{aligned}
q_{l,m} &= q\left[a^l Y^*_{l,m}(\theta=0,\varphi=0) - \cancelto{0}{20^l Y^*_{l,m}(\theta=0,\varphi=0)} + a^l Y^*_{l,m}(\theta=\pi,\varphi=0)\right] \\
&= qa^l\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\left[\underbrace{e^{im(0)}}_{1}P_l^m\left(\cos(0)\right) + \underbrace{e^{im(0)}}_{1}P_l^m\left(\cos(\pi)\right)\right] \\
&= qa^l\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\left[P_l^m(1) + P_l^m(-1)\right]
\end{aligned}
$$

Because we have azumuthal symmetry, only the $m=0$ terms survive. Noting that that $P_l^0(1)=1$, $P_l^0(-1)=(-1)^l$:

$$
\begin{aligned}
q_{l,m} &= qa^l\sqrt{\frac{(2l+1)}{4\pi}}\left[1+(-1)^l\right] \\
&= qa^l\sqrt{\frac{(2l+1)}{4\pi}}\begin{cases} 2 & l \text{ even}, m=0 \\ 0 & l \text{ odd OR } m\neq 0 \end{cases}
\end{aligned}
$$

$l=2$:

$$
q_{2,0} = qa^2\sqrt{\frac{5}{\pi}}
$$

$l=4$:

$$
q_{4,0} = qa^4\sqrt{\frac{9}{\pi}}
$$

Note that $q_{0,0}=0$. The formula we obtained for $q_{l,m}$ is only valid for $l\neq 0$ (0^0 is not necessarily zero).

1.3

Equation 4.1 in Jackson:

$$
\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}q_{l,m}\frac{Y_{l,m}(\theta,\varphi)}{r^{l+1}}
$$

Substituting in $q_{l,m}$ from part b:

$$\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0}\sum_{l=1}^{\infty}\frac{4\pi}{4l+1}\left(qa^{2l}\sqrt{\frac{(4l+1)}{4\pi}}\right)\frac{Y_{2l,0}(\theta,\varphi)}{r^{2l+1}}$$
$$= \frac{1}{4\pi\varepsilon_0}\sum_{l=1}^{\infty}\frac{4\pi}{4l+1}\left(qa^{2l}\sqrt{\frac{(4l+1)}{4\pi}}\right)\frac{\sqrt{\frac{(4l+1)}{4\pi}}P_{2l}^{0}(\cos\theta)}{r^{2l+1}}$$
$$= \frac{q}{4\pi\varepsilon_0}\sum_{l=1}^{\infty}a^{2l}\frac{P_{2l}(\cos\theta)}{r^{2l+1}}$$

The lowest-order ($l = 1$) term is:

$$\Phi(\vec{x}) = \frac{q}{4\pi\varepsilon_0}\frac{a^2}{r^3}\left(\frac{1}{2}\left(3\cos^2\theta - 1\right)\right) + \ldots$$

in the x-y plane, $\theta = \pi/2$:

$$\Phi_{x\text{-}y}(\vec{x}) = -\frac{q}{8\pi\varepsilon_0}\frac{a^2}{r^3}$$

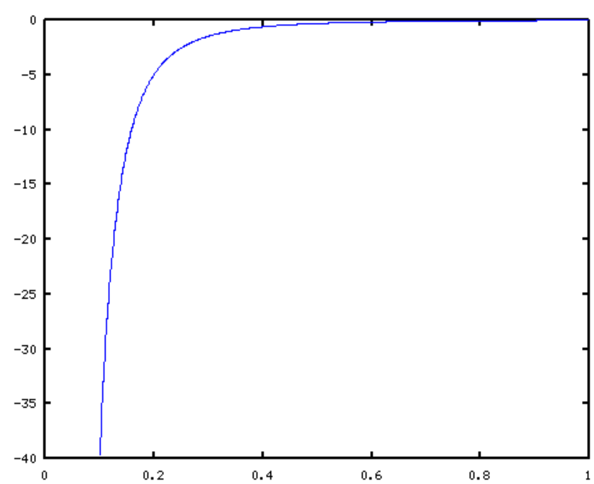

Figure 1:

1.4

$$\Phi = \frac{1}{4\pi\varepsilon_0}\frac{q}{\sqrt{r^2+a^2}} + \frac{1}{4\pi\varepsilon_0}\frac{q}{\sqrt{r^2+a^2}} - \frac{1}{4\pi\varepsilon_0}\frac{2q}{r}$$

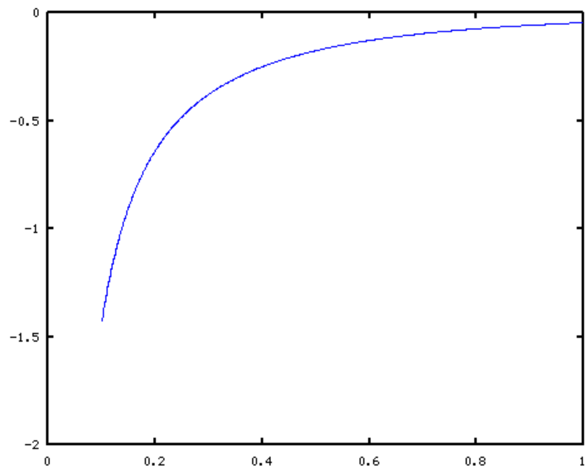

Figure 2:

The two plots have the same general shape. We don't expect them to be identical since the first figure represents a rough approximation.

2 Problem 4.7

2.1

Note:

$$\sin^2\theta = 1 - \cos^2\theta = \frac{2}{3}P_0^0(\cos\theta) - \frac{2}{3}P_2^0(\cos\theta)$$

Hence, $\rho(\vec{r})$ becomes:

$$\rho(\vec{r}) = \frac{1}{64\pi}\frac{2}{3}r^2e^{-r}\left(P_0^0(\cos\theta) - P_2^0(\cos\theta)\right) \tag{1}$$

Equation 4.3 in Jackson:

$$
\begin{aligned}
q_{l,m} &= \int Y^*_{l,m}(\theta',\varphi')r'^{l}\rho(\vec{x}')d^3x' \\
&= \iiint Y^*_{l,m}(\theta',\varphi')r'^{l}\left[\frac{1}{64\pi}\frac{2}{3}r'^2e^{-r'}\left(P^0_0(\cos\theta') - P^0_2(\cos\theta')\right)\right]r'^2\sin\theta' dr' d(\cos\theta')d\varphi' \\
&= \frac{1}{96\pi}\iiint r'^{4+l}e^{-r'}\left(P^0_0(\cos\theta') - P^0_2(\cos\theta')\right)Y^*_{l,m}(\theta',\varphi')dr'd(\cos\theta')d\varphi' \\
&= \frac{1}{96\pi}\iiint r'^{4+l}e^{-r'}\left(P^0_0(\cos\theta') - P^0_2(\cos\theta')\right)\left(\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P^m_l(\cos\theta)e^{im\varphi}\right)dr'd(\cos\theta')d\varphi' \\
&= \frac{1}{96\pi}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\iiint r'^{4+l}e^{-r'}e^{im\varphi}P^m_l(\cos\theta)\left(P^0_0(\cos\theta') - P^0_2(\cos\theta')\right)dr'd\cos(\theta')d\varphi' \\
&= \frac{1}{96\pi}\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\iiint r'^{4+l}e^{-r'}e^{im\varphi}P^m_l(\cos\theta)\left(P^0_0(\cos\theta') - P^0_2(\cos\theta')\right)dr'd(\cos\theta')d\varphi'
\end{aligned}
$$

By orthogonality, only the $m = 0$, $l = 0, 2$ terms survive. Because $\int [P_0(x)]^2\,dx = 2$ and $\int [P_2(x)]^2\,dx = \frac{2}{5}$:

$$
q_{l,m} = \frac{1}{96\pi}\sqrt{\frac{(2l+1)}{4\pi}}\iint r'^{4+l}e^{-r'}e^{i(0)\varphi}dr'd\varphi' \times \begin{cases} 2 & l = 0 \\ -\frac{2}{5} & l = 2 \end{cases}
$$

The integral evaluates to:

$$
\int_{\varphi'=0}^{2\pi}\int_{r'=0}^{\infty} r'^{4+l}e^{-r'}dr'd\varphi' = 2\pi\int_{r'=0}^{\infty} r'^{4+l}e^{-r'}dr'd\varphi' = 2\pi\Gamma(l+5) = 2\pi(l+4)!
$$

where Maple command `int(r^(4+l)*exp(-r),r=0..infinity);` was used to evaluate the last integral. Thus,

$$
q_{l,0} = \frac{1}{96}\sqrt{\frac{1}{\pi}}\begin{cases} 4! & l = 0 \\ -\sqrt{5}\cdot 6! & l = 2 \\ 0 & \text{otherwise} \end{cases}
$$

Specifically,

$$
\begin{aligned}
q_{0,0} &= \frac{1}{2}\sqrt{\frac{1}{\pi}} \\
q_{2,0} &= -6\sqrt{\frac{5}{\pi}}
\end{aligned}
$$

Plugging this into equation 4.1 in Jackson:

$$\begin{aligned}
\Phi(\vec{x}) &= \frac{1}{4\pi\varepsilon_0}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{4\pi}{2l+1}q_{l,m}\frac{Y_{l,m}(\theta,\varphi)}{r^{l+1}} \\
&= \frac{1}{4\pi\varepsilon_0}4\pi\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right)\frac{Y_{0,0}(\theta,\varphi)}{r} + \frac{1}{4\pi\varepsilon_0}\frac{4\pi}{5}\left(-6\sqrt{\frac{5}{\pi}}\right)\frac{Y_{2,0}(\theta,\varphi)}{r^3} \\
&= \frac{1}{2\varepsilon_0 r\sqrt{\pi}}\left(\frac{1}{2}\sqrt{\frac{1}{\pi}}\right) - \frac{6}{5\varepsilon_0 r^3}\sqrt{\frac{5}{\pi}}\left(\frac{1}{2}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta - 1\right)\right) \\
&= \frac{1}{4\pi\varepsilon_0 r} - \frac{6}{4\pi\varepsilon_0 r^3}\underbrace{\left(3\cos^2\theta - 1\right)}_{2P_2(\cos\theta)}
\end{aligned}$$

$$\boxed{\Phi(\vec{x}) = \frac{1}{4\pi\varepsilon_0 r} - \frac{3}{2\pi\varepsilon_0 r^3}P_2(\cos\theta)}$$

2.2

Because we have no conducting surfaces, the Green function is simply:

$$G_D = \frac{1}{|\vec{r}-\vec{r}'|} = \sum_l \frac{r_<^l}{r_>^{l+1}}P_l(\cos\theta')P_l(\cos\theta) \tag{2}$$

Note that we have azimuthal symmetry due to having no surfaces.

We only need to consider the first integral in equation 1.44 in Jackson (since we have no surfaces):

$$\Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int \rho(\vec{r}')G_D(\vec{r},\vec{r}')d^3r'$$

Plugging in equation (2) for $G_D(\vec{r},\vec{r}')$ and equation (1) for $\rho(\vec{r}')$:

$$\Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\iiint\sum_l \frac{r_<^l}{r_>^{l+1}}P_l(\cos\theta')P_l(\cos\theta)\left[\frac{1}{64\pi}\frac{2}{3}r'^2e^{-r'}\left(P_0(\cos\theta') - P_2(\cos\theta')\right)\right]r'^2dr'd(\cos\theta)d\varphi$$

By orthogonality, only the $l = 0, 2$ terms survive. $\int\left[P_0(x)\right]^2dx = 2$ and $\int\left[P_2(x)\right]^2dx = \frac{2}{5}$:

$$\Phi(\vec{r}) = \frac{1}{384\pi^2\varepsilon_0}P_l(\cos\theta)\iint\frac{r_<^l}{r_>^{l+1}}r'^4e^{-r'}dr'd\varphi \times \begin{cases}2 & l=0\\ -\frac{2}{5} & l=2\end{cases}$$

The integral evaluates to:

$$\begin{aligned}\int_{\varphi'=0}^{2\pi}\int_{r'=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}r'^4e^{-r'}\,dr'd\varphi &= 2\pi\int_{r'=0}^{\infty}\frac{r_<^l}{r_>^{l+1}}r'^4e^{-r'}\,dr' \\ &= 2\pi\int_{r'=0}^{r}\frac{r'^l}{r^{l+1}}r'^4e^{-r'}\,dr' + 2\pi\int_{r'=r}^{\infty}\frac{r^l}{r'^{l+1}}r'^4e^{-r'}\,dr' \\ &= \frac{2\pi}{r^{l+1}}\int_{r'=0}^{r}r'^{l+4}e^{-r'}\,dr' + 2\pi r^l\int_{r'=r}^{\infty}r'^{3-l}e^{-r'}\,dr'\end{aligned}$$

$$= \begin{cases} -2\pi\left[e^{-r}\left(r^2+6r+18+24r^{-1}\right)-24r^{-1}\right] & l=0 \\ -10\pi\left[e^{-r}\left(r^2+6r+24r+72r^{-1}+144r^{-2}+144r^{-3}\right)-144r^{-3}\right] & l=2 \end{cases}$$

Plugging this back into $\Phi(\vec{r})$:

$$\begin{aligned}\Phi(\vec{r}) = &-\frac{P_0(\cos\theta)}{96\pi\varepsilon_0}\left[e^{-r}\left(r^2+6r+18+24r^{-1}\right)-24r^{-1}\right] \\ &+\frac{P_2(\cos\theta)}{96\pi\varepsilon_0}\left[e^{-r}\left(r^2+6r+24r+72r^{-1}+144r^{-2}+144r^{-3}\right)-144r^{-3}\right]\end{aligned}$$

For small r, this reduces to:

$$\Phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\left[\frac{1}{4}-\frac{r^2}{120}P_2(\cos\theta)\right]$$

2.3

Near the nucleus Φ is as we found at the end of part b multiplied by the electron charge e.

The interaction energy is found using equation 4.21 in Jackson:

$$\begin{aligned}
W &= \int \rho(\vec{r})\Phi(\vec{r})d^3r \\
&= \int \rho(\vec{r})\frac{1}{4\pi\varepsilon_0}\left[\frac{1}{4} - \frac{r^2}{120}P_2(\cos\theta)\right] d^3r \\
&= \frac{1}{16\pi\varepsilon_0}\int \rho(\vec{r})d^3r - \frac{1}{480\pi\varepsilon_0}\int r^2 P_2(\cos\theta)\rho(\vec{r})d^3r \\
&= \frac{1}{16\pi\varepsilon_0}\int \rho(\vec{r})d^3r - \frac{1}{480\pi^2\varepsilon_0}\int r^2\left[\frac{1}{2}\left(3\cos^2\theta - 1\right)\right]\rho(\vec{r})d^3r \\
&= \frac{1}{16\pi\varepsilon_0}\int \rho(\vec{r})d^3r - \frac{1}{960\pi^2\varepsilon_0}\int \left(3\underbrace{r^2\cos^2\theta}_{z^2} - r^2\right)\rho(\vec{r})d^3r \\
&= \frac{1}{16\pi\varepsilon_0}\underbrace{\int \rho(\vec{r})d^3r}_{e} - \frac{1}{960\pi^2\varepsilon_0}\underbrace{\int \left(3z^2 - r^2\right)\rho(\vec{r})d^3r}_{Q_{z,z}}
\end{aligned}$$

where we have used the definition of the quadrupole moment tensor (equation 4.9 in Jackson). Since we are given that $Q_{i,i} = (e/a_0^3)\cdot 10^{-28}\ \mathrm{m}^3$:

$$W = \frac{1}{16\pi\varepsilon_0}e - \frac{1}{960\pi^2\varepsilon_0}\frac{e}{a_0^3}\cdot 10^{-28}\ \mathrm{m}^3$$

$$\frac{W}{h} = \frac{e}{h}\left(\frac{1}{16\pi\varepsilon_0} - \frac{10^{-28}\ \mathrm{m}^3}{960\pi^2\varepsilon_0 a_0^3}\right)$$