PH415 : Homework 9

(Post_Midsem Homework 4)

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$$\rho_a(\overline{r}) = Ze\,\delta^3(\overline{r}) - \frac{Ze}{8\pi\,\xi^3}\,e^{-\frac{|\overline{r}|}{\xi}}$$
$$= \rho_a{}^{(n)} + \rho_a{}^{(e)}$$

$$\rho_b(\overline{r}') = Ze\,\delta^3(\overline{r}' - R\,\widehat{z}) - \frac{Ze}{8\pi\,\xi^3}\,e^{-\frac{|\overline{r}' - R\,\widehat{z}|}{\xi}}$$
$$= \rho_b{}^{(n)} + \rho_b{}^{(e)}$$

$$I = \int d^3\overline{r} \int d^3\overline{r}'\,\frac{\rho_a(\overline{r})\,\rho_b(\overline{r}')}{|\overline{r} - \overline{r}'|}$$
$$= I_1 + I_2 + I_3 + I_4$$
$$= I^{(n-n)} + I^{(n-e)} + I^{(e-n)} + I^{(e-e)}$$

$$I_1 = \int d^3\overline{r} \int d^3\overline{r}'\,\frac{\rho_a{}^{(n)}(\overline{r})\,\rho_b{}^{(n)}(\overline{r}')}{|\overline{r} - \overline{r}'|}$$
$$= (Ze)^2 \int d^3\overline{r} \int d^3\overline{r}'\,\frac{\delta^3(\overline{r})\,\delta^3(\overline{r}' - R\,\widehat{z})}{|\overline{r} - \overline{r}'|}$$
$$= \frac{(Ze)^2}{|\overline{0} - R\,\widehat{z}|}$$

$$I_1 = \frac{(Ze)^2}{R}$$

$$I_2 = \int d^3\overline{r} \int d^3\overline{r}'\,\frac{\rho_a{}^{(n)}(\overline{r})\,\rho_b{}^{(e)}(\overline{r}')}{|\overline{r} - \overline{r}'|}$$
$$= -\frac{(Ze)^2}{8\pi\,\xi^3} \int d^3\overline{r} \int d^3\overline{r}'\,\frac{\delta^3(\overline{r})\,e^{-\frac{|\overline{r}' - R\,\widehat{z}|}{\xi}}}{|\overline{r} - \overline{r}'|}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\bar{r}'\,\frac{e^{-\frac{|\bar{r}'-R\,\hat{z}|}{\xi}}}{|\bar{0}-\bar{r}'|}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int dr'\int d\theta'\int d\phi'\,\frac{r'^2\sin(\theta')}{r'}\,e^{-\frac{\sqrt{r'^2+R^2-2r'R\cos(\theta')}}{\xi}}$$

$$I_2 = -\frac{(Ze)^2}{R}\left[1-e^{-R/\xi}\left(1+\frac{R}{2\,\xi}\right)\right]$$

$$I_3 = \int d^3\bar{r}\int d^3\bar{r}'\,\frac{\rho_a{}^{(e)}(\bar{r})\,\rho_b{}^{(n)}(\bar{r}')}{|\bar{r}-\bar{r}'|}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\bar{r}\int d^3\bar{r}'\,\frac{\delta^3(\bar{r}'-R\,\hat{z})\,e^{-\frac{|\bar{r}|}{\xi}}}{|\bar{r}-\bar{r}'|}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\bar{r}\,\frac{e^{-\frac{|\bar{r}|}{\xi}}}{|\bar{r}-R\,\hat{z}|}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int dr\int d\theta\int d\phi\,\frac{r^2\sin(\theta)}{\sqrt{r^2+R^2-2rR\cos(\theta)}}\,e^{-\frac{r}{\xi}}$$

$$I_3 = -\frac{(Ze)^2}{R}\left[1-e^{-R/\xi}\left(1+\frac{R}{2\,\xi}\right)\right]$$

$$I_4 = \int d^3\bar{r}\int d^3\bar{r}'\,\frac{\rho_a{}^{(e)}(\bar{r})\,\rho_b{}^{(e)}(\bar{r}')}{|\bar{r}-\bar{r}'|}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\bar{r}\int d^3\bar{r}'\,\frac{e^{-\frac{|\bar{r}|}{\xi}}\,e^{-\frac{|\bar{r}'-R\,\hat{z}|}{\xi}}}{|\bar{r}-\bar{r}'|}$$

Now,

$$\frac{1}{|\bar{r}-\bar{r}'|} = \frac{1}{\sqrt{r^2+r'^2-2\,r\,r'\cos(\gamma)}}$$, where $\gamma = (\theta-\theta')$

$$= \frac{1}{r_>}\left(1+\frac{r_<^2}{r_>^2}-\frac{2r_<}{r_>}\cos(\gamma)\right)^{-1/2} \quad \text{, where} \quad \begin{aligned} r_< &= \min(r,r') \\ r_> &= \max(r,r') \end{aligned}$$

$$= \frac{1}{r_>}\sum_{l=0}^{\infty}\left(\frac{r_<}{r_>}\right)^{l} P_l(\cos(\gamma))$$

$$= 4\pi\sum_{l=0}^{\infty}\frac{1}{2l+1}\frac{r_<^l}{r_>^{l+1}}\sum_{m=-l}^{l} Y_l^m(\theta,\phi)\, Y_l^m(\theta',\phi')^*$$

Putting this expansion of $\dfrac{1}{|\overline{r}-\overline{r}'|}$ in Integral I_4, we get:

$$I_4 = -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\overline{r}'\, e^{-\frac{|\overline{r}'-R\,\hat{z}|}{\xi}} \underbrace{\left[\int d^3\overline{r}\,\frac{e^{-\frac{|\overline{r}|}{\xi}}}{|\overline{r}-\overline{r}'|}\right]}_{I_{4r}}$$

$$\int d^3\overline{r}\,\frac{e^{-\frac{|\overline{r}|}{\xi}}}{|\overline{r}-\overline{r}'|} = 4\pi\sum_{l=0}^{\infty}\frac{1}{2l+1}\int_0^{\infty} dr\int_0^{\pi} d\theta\int_0^{2\pi} d\phi\, e^{-r/\xi}\, r^2\sin(\theta)\frac{r_<^l}{r_>^{l+1}}\sum_{m=-l}^{l} Y_l^m(\theta,\phi)\, Y_l^m(\theta',\phi')^*$$

From the definition of Spherical Harmonics,

$$\int_0^{\pi} d\theta\int_0^{2\pi} d\phi\,\sin(\phi)\, Y_l^m(\theta,\phi)\, Y_{l'}^{m'}(\theta,\phi) = \delta_{ll'}\delta_{mm'}$$

$$\Longrightarrow \int_0^{\pi} d\theta\int_0^{2\pi} d\phi\,\sin(\phi)\, Y_l^m(\theta,\phi)\, Y_0^0(\theta,\phi) = \delta_{l0}\delta_{m0}$$

$$\Longrightarrow \int_0^{\pi} d\theta\int_0^{2\pi} d\phi\,\sin(\phi)\, Y_l^m(\theta,\phi)\,\frac{1}{\sqrt{4\pi}} = \delta_{l0}\delta_{m0}$$

$$\Longrightarrow \int_0^{\pi} d\theta\int_0^{2\pi} d\phi\,\sin(\phi)\, Y_l^m(\theta,\phi) = \sqrt{4\pi}\,\delta_{l0}\delta_{m0}$$

$$= 4\pi\int_0^{\infty} dr\, e^{-r/\xi}\, r^2\,\frac{r_<^0}{r_>^{0+1}}\sqrt{4\pi}\, Y_0^0(\theta',\phi')^*$$

$$= 4\pi\int_0^{\infty} dr\, e^{-r/\xi}\,\frac{r^2}{r_>}\sqrt{4\pi}\left(\frac{1}{\sqrt{4\pi}}\right)$$

$$= 4\pi\left(\frac{1}{r'}\int_0^{r'} dr\, e^{-r/\xi}\, r^2 + \int_{r'}^{\infty} dr\, e^{-r/\xi}\, r\right)$$

$$= 4\pi\left\{\frac{1}{r'}\left[2\xi^2 - e^{-r'/\xi}\xi\left(2\xi^2 + 2\xi r' + r'^2\right)\right] + \left[e^{-r'/\xi}\xi(r'+\xi)\right]\right\}$$

$$= \frac{8\pi\xi^3}{r'}\left[1 - e^{-r'/\xi}\left(1 + \frac{r'}{2\xi}\right)\right]$$

$$:= I_{4r}$$

Substituting this value of I_{4r}, in equation of I_4, we get:

$$I_4 = -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\overline{r}'\, e^{-\frac{|\overline{r}' - R\,\hat{z}|}{\xi}} \underbrace{\left[\int d^3\overline{r}\, \frac{e^{-\frac{|\overline{r}|}{\xi}}}{|\overline{r} - \overline{r}'|}\right]}_{I_{4r}}$$

$$= -\frac{(Ze)^2}{8\pi\,\xi^3}\int d^3\overline{r}'\, e^{-\frac{|\overline{r}' - R\,\hat{z}|}{\xi}}\, \frac{8\pi\xi^3}{r'}\left[1 - e^{-r'/\xi}\left(1 + \frac{r'}{2\xi}\right)\right]$$

$$= -(Ze)^2\int d^3\overline{r}'\, \frac{e^{-\frac{|\overline{r}' - R\,\hat{z}|}{\xi}}}{r'}\left[1 - e^{-r'/\xi}\left(1 + \frac{r'}{2\xi}\right)\right]$$

$$= -(Ze)^2\int_0^{\infty} dr'\int_0^{\pi} d\theta'\int_0^{2\pi} d\phi'\, r'^2\sin(\theta')\, \frac{e^{-\frac{\sqrt{r'^2 + R^2 - 2r'R\cos(\theta')}}{\xi}}}{r'}\left[1 - e^{-r'/\xi}\left(1 + \frac{r'}{2\xi}\right)\right]$$

$$= -(Ze)^2(2\pi)\int_0^{\infty} dr'\int_0^{\pi} d\theta'\, \sin(\theta')\, r' e^{-\frac{\sqrt{r'^2 + R^2 - 2r'R\cos(\theta')}}{\xi}}\left[1 - e^{-r'/\xi}\left(1 + \frac{r'}{2\xi}\right)\right]$$

This involves integral of the form $\int_0^{\pi} d\theta' \sin(\theta')\, e^{-\frac{\sqrt{a-b\cos(\theta')}}{c}}$, where $\begin{matrix} a,b,c>0 \\ a \geqslant b \end{matrix}$

$$\int_0^{\pi} d\theta' \sin(\theta')\, e^{-\frac{\sqrt{a-b\cos(\theta')}}{c}} = 2\frac{c}{b}\, e^{-\frac{\sqrt{a-b}+\sqrt{a+b}}{c}} \times \ldots$$

$$\left[-\left(\sqrt{a+b}+c\right)e^{\frac{\sqrt{a-b}}{c}} + \left(\sqrt{a-b}+c\right)e^{\frac{\sqrt{a+b}}{c}}\right]$$

$$\Longrightarrow \int_0^{\pi} d\theta' \sin(\theta')\, e^{-\frac{\sqrt{r'^2+R^2-2r'R\cos(\theta')}}{\xi}} = \ldots$$

$$\begin{cases} e^{-(r'+R)/\xi}\, \dfrac{\xi}{r'R}\left[e^{2r'/\xi}(-r'+R+\xi)-(r'+R+\xi)\right] & r' \leqslant R \\ e^{-(r'+R)/\xi}\, \dfrac{\xi}{r'R}\left[e^{2R/\xi}(r'-R+\xi)-(r'+R+\xi)\right] & r' \geqslant R \end{cases}$$

$$I_4 = -(Ze)^2(2\pi)\,\frac{\xi}{R}\int_0^R dr' e^{-(r'+R)/\xi}\left[e^{2r'/\xi}(-r'+R+\xi)-(r'+R+\xi)\right]\left[1-e^{-r'/\xi}\left(1+\frac{r'}{2\xi}\right)\right]$$

$$+-(Ze)^2(2\pi)\,\frac{\xi}{R}\int_R^{\infty} dr' e^{-(r'+R)/\xi}\left[e^{2R/\xi}(r'-R+\xi)-(r'+R+\xi)\right]\left[1-e^{-r'/\xi}\left(1+\frac{r'}{2\xi}\right)\right]$$

$$= -(Ze)^2(2\pi)\,\frac{\xi}{R}\,(I_{<R} + I_{>R}), \quad \text{where :}$$

$$I_{<R} = 2\xi^2 - \frac{1}{8}e^{-\frac{3R}{\xi}}\left(8\xi^2+4R^2+13\xi R\right) - \frac{e^{-\frac{R}{\xi}}\left(72\xi^3+18\xi R^2+2R^3+57\xi^2 R\right)}{24\xi} + 2\xi e^{-\frac{2R}{\xi}}(\xi+R)$$

and

$$I_{>R} = 2\xi^2 + e^{-\frac{3R}{\xi}}\left(\xi^2+\frac{R^2}{2}+\frac{13\xi R}{8}\right) - 2\xi e^{-\frac{2R}{\xi}}(\xi+R) - \frac{1}{8}\xi e^{-\frac{R}{\xi}}(8\xi+3R)$$

$$\Longrightarrow I_4 = -(Ze)^2(2\pi)\,\frac{\xi}{R}\left(4\xi^2 - \frac{e^{-\frac{R}{\xi}}\left(48\xi^3+9\xi R^2+R^3+33\xi^2 R\right)}{12\xi}\right)$$

$$I_4 = -\left(8\pi\xi^3\right)\frac{(Ze)^2}{R}\left[1 - e^{-R/\xi}\left(\frac{R^3}{48\xi^3} + \frac{3R^2}{16\xi^2} + \frac{11R}{16\xi} + 1\right)\right]$$

Adding these 4 integrals, we get finally :

$$I = I_1 + I_2 + I_3 + I_4$$

$$I = \frac{(Ze)^2}{R} - 2\frac{(Ze)^2}{R}\left[1 - e^{-R/\xi}\left(1 + \frac{R}{2\,\xi}\right)\right] \ldots$$
$$- \left(8\pi\xi^3\right)\frac{(Ze)^2}{R}\left[1 - e^{-R/\xi}\left(\frac{R^3}{48\xi^3} + \frac{3R^2}{16\xi^2} + \frac{11R}{16\xi} + 1\right)\right]$$