3.012 Bonding-Structure: Recitation 3 (Solutions)

1 Spherical Harmonics

Solution I

From what is already given and from the knowledge of some of the simplest spherical harmonics (such as the $s = Y_{00}$), one might conjecture that:
- the number of vertical nodal planes is m;
- the total number of nodal surfaces is l.

The distinction between real part, $\mathrm{Re}(Y_{lm})$, and imaginary part, $\mathrm{Im}(Y_{lm})$, is more difficult. The rule is following: $\mathrm{Im}(Y_{lm})$ always corresponds to cases where one of the vertical nodal surfaces contains the x-axis.

$$Y_{lm} : \left\{ \begin{array}{rcr} \text{number of vertical nodal planes} & : & m \\ + \text{ number of other nodal surfaces} & : & l-m \\ \hline \text{total number of nodal surfaces} & : & l \end{array} \right.$$

2 Radial Functions, R_{nl}

Solution II

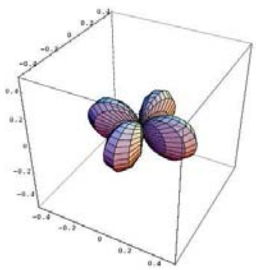
We already know that the number of radial nodes (nodal spheres) is $n - l - 1$ (Lecture 7).

Moreover, it can be observed that the radial wavefunction behaves as r^l when r goes to zero (the first term in the Taylor expansion of $R_{nl}(r)$ around $r = 0$ is proportional to r^l).

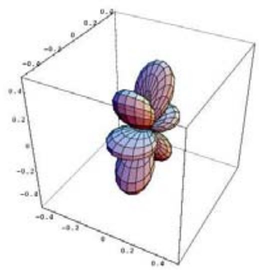
$$R_{nl} : \left\{ \begin{array}{rcr} \text{total number of nodes } (r = 0 \text{ no taken into account}) & : & n-l-1 \\ \text{behaviour at the origin} & : & R_{nl}(r) \text{ behaves as } r^l \end{array} \right.$$

The total number of nodes (angular and radial) for $Y_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi)$ is thus:

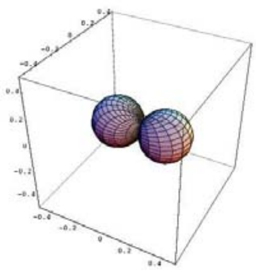
$(n - l - 1) + (m - l) + (m) = n - 1$.



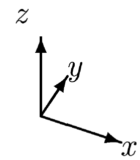
(a) $\mathrm{Re}(Y_{l=2,m=2})$ $d_{x^2-y^2}$

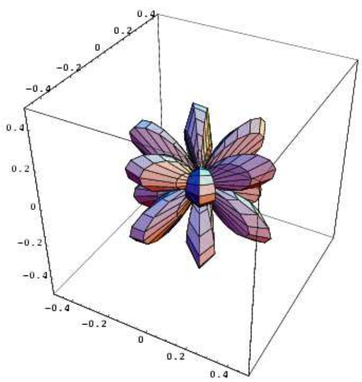


(b) $\mathrm{Im}(Y_{l=3,m=1})$

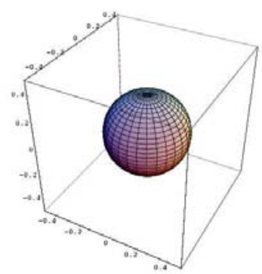


(c) $\mathrm{Re}(Y_{l=1,m=1})$ p_x

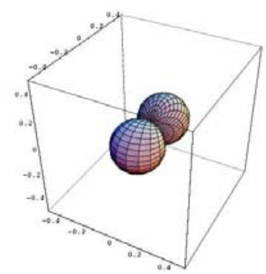




(d) $\mathrm{Re}(Y_{l=4,m=3})$

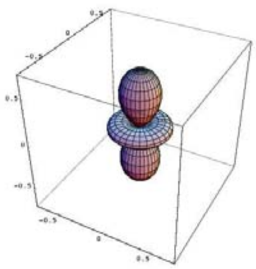


(e) $\mathrm{Re}(Y_{l=0,m=0})$ s

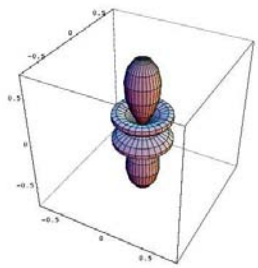


(f) $\mathrm{Im}(Y_{l=1,m=1})$ p_y

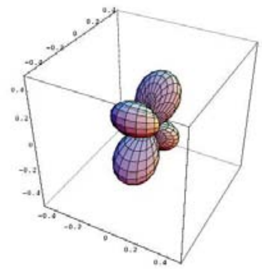
Figure 1: Spherical Harmonics



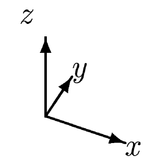
(a) $\mathrm{Re}(Y_{l=2,m=0})$ d_{z^2}

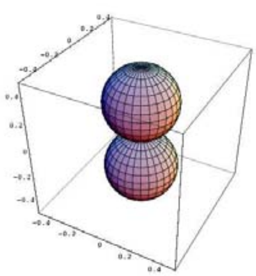


(b) $\mathrm{Re}(Y_{l=3,m=0})$

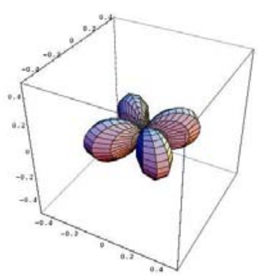


(c) $\mathrm{Im}(Y_{l=2,m=1})$ d_{yz}

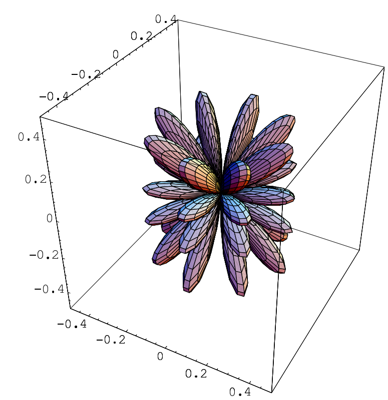




(d) $\mathrm{Re}(Y_{l=1,m=0})$ p_z

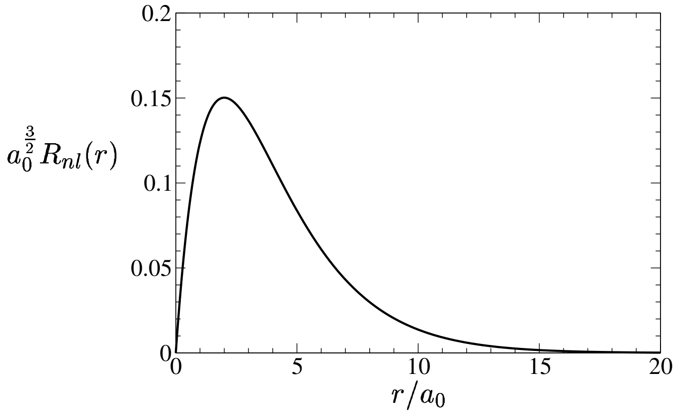


(e) $\mathrm{Im}(Y_{l=2,m=2})$ d_{xy}

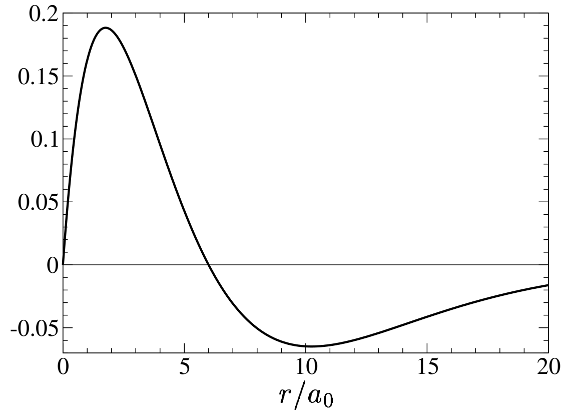


(f) $\mathrm{Re}(Y_{l=7,m=4})$

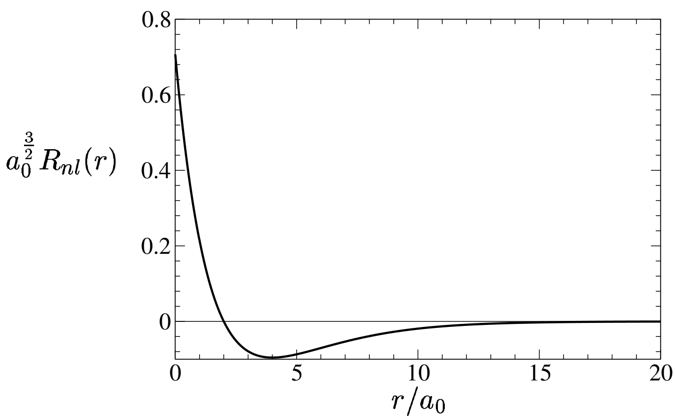
Figure 2: Spherical Harmonics



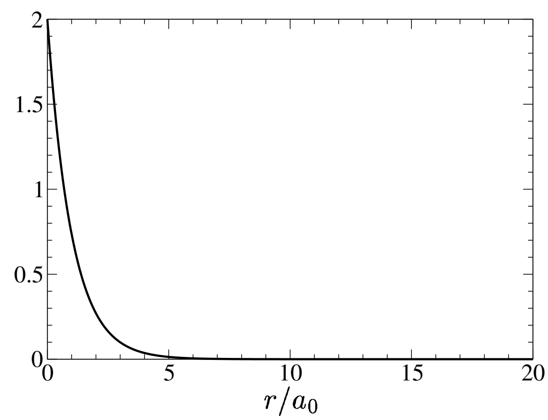
(a) $R_{n=2,l=1}$



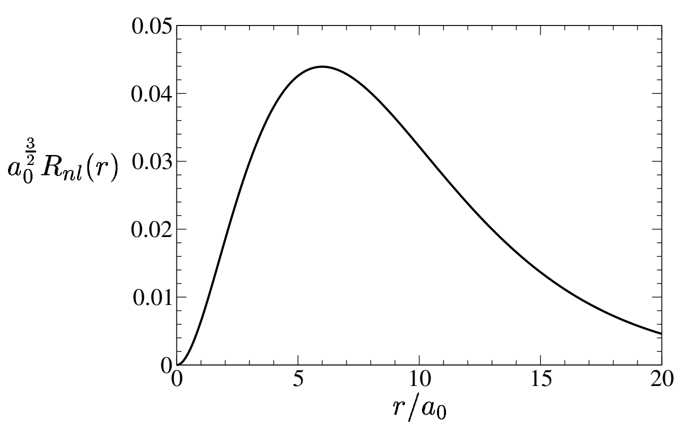
(b) $R_{n=3,l=1}$



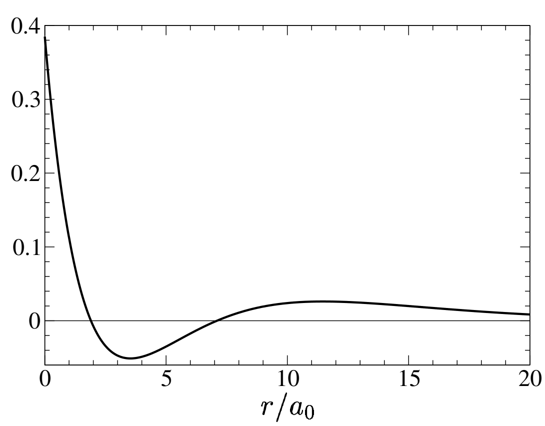
(c) $R_{n=2,l=0}$



(d) $R_{n=1,l=0}$



(e) $R_{n=3,l=2}$



(f) $R_{n=3,l=0}$

Figure 3: Radial Functions