1 Orbitaly atomu vodíku - radiální části

$$a = \frac{\hbar^2}{\gamma m_e} \qquad V = -\frac{\gamma}{r}$$

$$R_{10}(r) = \frac{2}{a^{3/2}} \exp\left(-\frac{r}{a}\right)$$

$$R_{20}(r) = \frac{1}{(2a^3)^{1/2}} \left(1 - \frac{r}{2a}\right) \exp\left(-\frac{r}{2a}\right)$$

$$R_{21}(r) = \frac{1}{2(6a^3)^{1/2}} \left(\frac{r}{a}\right) \exp\left(-\frac{r}{2a}\right)$$

$$R_{30}(r) = \frac{2}{3(3a^3)^{1/2}} \left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right) \exp\left(-\frac{r}{3a}\right)$$

$$R_{31}(r) = \frac{4}{27} \left(\frac{2}{3a^3}\right)^{1/2} \left(\frac{r}{a}\right) \left(1 - \frac{1}{6}\frac{r}{a}\right) \exp\left(-\frac{r}{3a}\right)$$

$$R_{32}(r) = \frac{2}{81} \left(\frac{2}{15a^3}\right)^{1/2} \left(\frac{r}{a}\right)^2 \exp\left(-\frac{r}{3a}\right)$$

$$R_{40}(r) = \frac{1}{4a^3/2} \left(1 - \frac{3}{4}\frac{r}{a} + \frac{1}{8}\left(\frac{r}{a}\right)^2 - \frac{1}{192}\left(\frac{r}{a}\right)^3\right) \exp\left(-\frac{r}{4a}\right)$$

$$R_{41}(r) = \frac{1}{16} \left(\frac{5}{3a^3}\right)^{1/2} \left(\frac{r}{a}\right) \left(1 - \frac{1}{4}\frac{r}{a} + \frac{1}{80}\left(\frac{r}{a}\right)^2\right) \exp\left(-\frac{r}{4a}\right)$$

$$R_{42}(r) = \frac{1}{64} \left(\frac{1}{5a^3}\right)^{1/2} \left(\frac{r}{a}\right)^2 \left(1 - \frac{1}{12}\frac{r}{a}\right) \exp\left(-\frac{r}{4a}\right)$$

$$R_{43}(r) = \frac{1}{768} \left(\frac{1}{35a^3}\right)^{1/2} \left(\frac{r}{a}\right)^3 \exp\left(-\frac{r}{4a}\right)$$

2 Vlastní funkce momentu hybnosti (sférické harmoniky)

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$$

$$Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}} \mathrm{e}^{\pm\mathrm{i}\phi} \sin\theta = \mp\sqrt{\frac{3}{8\pi}} \frac{x \pm \mathrm{i}y}{r}$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1) = \sqrt{\frac{5}{16\pi}} \frac{3z^2 - r^2}{r^2}$$

$$Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}} \mathrm{e}^{\pm\mathrm{i}\phi} \sin\theta\cos\theta = \mp\sqrt{\frac{15}{8\pi}} \frac{(x \pm \mathrm{i}y)z}{r^2}$$

$$Y_{2,\pm2} = \mp\sqrt{\frac{15}{32\pi}} \mathrm{e}^{\pm2\mathrm{i}\phi} \sin^2\theta = \mp\sqrt{\frac{15}{32\pi}} \frac{x^2 - y^2 \pm 2\mathrm{i}xy}{r^2}$$

3 Maticové elementy $\langle nlm|r^s|nlm\rangle$ pro orbitaly atomu vodíku

$$\langle nlm|r^2|nlm\rangle = a^2n^2(5n^2+1-3l(l+1))/2$$

$$\langle nlm|r|nlm\rangle = a(3n^2-l(l+1))/2$$

$$\langle nlm|nlm\rangle = 1$$

$$\langle nlm|r^{-1}|nlm\rangle = a^{-1}n^{-2}$$

$$\langle nlm|r^{-2}|nlm\rangle = a^{-2}(n^3(l+1/2))^{-1}$$