13) a)

$$\langle \vec{L}^2 \rangle = l(l+1)\hbar^2 \qquad \text{mit} \quad l = 0, 1, 2, \ldots, n-1$$

$$\langle L_z \rangle = m\hbar \qquad \text{mit} \quad m = 0, \pm 1, \pm 2, \ldots, \pm l$$

$n = 5$ $\quad l = 0 \quad m = 0$

$\quad l = 1 \quad m = 0, \pm 1$

$\quad l = 2 \quad m = 0, \pm 1, \pm 2$

$\quad \vdots$

$\quad l = 4 \quad m = 0, \pm 1, \pm 2, \pm 3, \pm 4$

$n = 6$ $\quad l = 0 \quad m = 0$

$\quad \vdots$

$\quad l = 5 \quad m = 0, \pm 1, \pm 2, \ldots \pm 5$

b) $$R_{1,0}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr}{a_0}} \overset{Z=1}{=} 2\left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{r}{a_0}}$$

$\Rightarrow$ kein Nullstelle!

$$R_{2,0}(r) \overset{Z=1}{=} 2\left(\frac{1}{2a_0}\right)^{3/2}\left(1 - \frac{r}{2a_0}\right)\cdot e^{-\frac{r}{2a_0}}$$

Nullstelle $r_0 = 2a_0$

c) $\int_r^{r+\Delta r} r^2 R_{n,l}^2(r)\,dr \;\hat{=}$ Aufenthaltswahrscheinlichkeit des Elektrons in einer Kugelschale vom Radius r und Dicke Δr

$n = 1$

$$\int_0^\infty r^2 R_{n,l}^2(r)\,dr = \int_0^\infty r^2 R_{1,0}^2(r)\,dr$$

muß natürlich 1 ergeben (Normierung: irgendwo ist das Elektron)

Rechnung:

$$= \int_0^\infty r^2\, 4\left(\frac{1}{a_0}\right)^3 e^{-\frac{2r}{a_0}}\,dr$$

$$= 4\left(\frac{1}{a_0}\right)^3 \int_0^\infty r^2 e^{-\frac{2}{a_0}r}\,dr$$

Bronstein

$$= 4\left(\frac{1}{a_0}\right)^3 \left[e^{-\frac{2}{a_0}r} \cdot \left(\frac{r^2}{-\frac{2}{a_0}} - \frac{2r}{\frac{4}{a_0^2}} + \frac{2}{-\frac{8}{a_0^3}} \right) \right] \Bigg|_0^\infty$$

$$= \frac{4}{a_0^3} \cdot \left(0 - \frac{2}{-\frac{8}{a_0^3}} \right) = 1$$

d)

$n = 1$

$$r^2 R_{1,0}^2(r) = r^2 \frac{4}{a_0^3} e^{-\frac{2r}{a_0}}$$

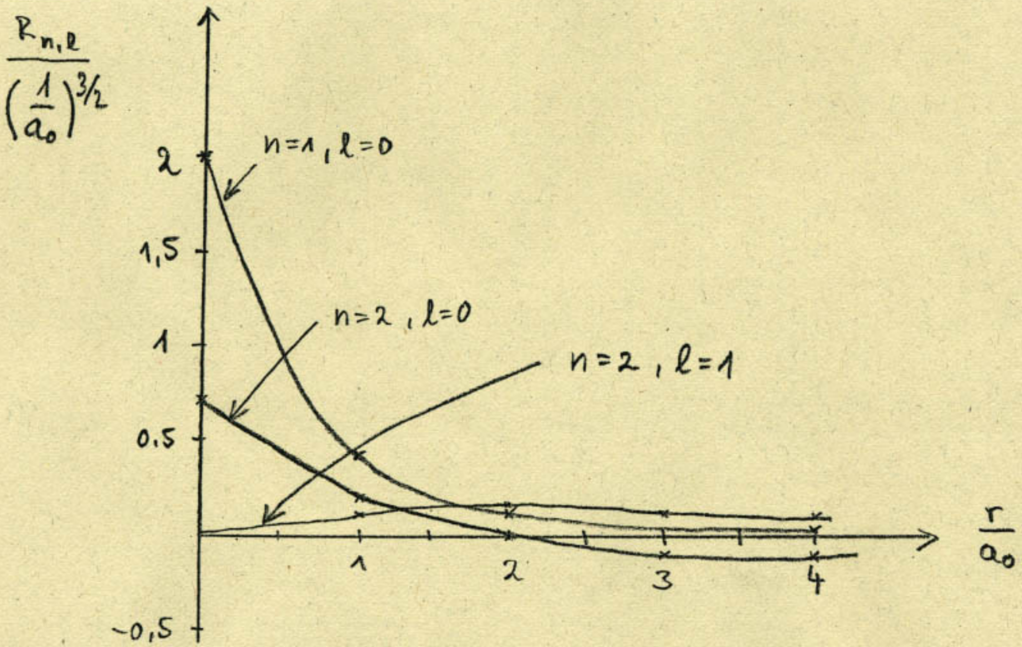
$$\frac{d}{dr}\left(r^2 R_{1,0}^2(r)\right)$$

$$= \frac{4}{a_0^3}\left(2r\, e^{-\frac{2r}{a_0}} - \frac{2r^2}{a_0} e^{-\frac{2r}{a_0}}\right) \overset{!}{=} 0$$

$$\Rightarrow r_1 = 0 \;,\; r_2 = a_0$$

$$R_{2,1} = \frac{2}{\sqrt{3}} \left(\frac{1}{2a_0} \right)^{3/2} \frac{r}{2a_0} e^{-\frac{r}{2a_0}}$$

$\Rightarrow$ Nullstelle $r_0 = 0$



$n=2,\ l=0$

$$\frac{d}{dr}\left(r^2 R_{2,0}^2(r)\right) = \frac{d}{dr}\left(r^2 \frac{1}{2a_0^3}\left(1-\frac{r}{2a_0}\right)^2 e^{-\frac{r}{a_0}}\right)$$

$$= \frac{1}{2a_0^3}\left\{2\left(r-\frac{r^2}{2a_0}\right)\left(1-\frac{2r}{2a_0}\right) - \frac{1}{a_0}\left(r-\frac{r^2}{2a_0}\right)^2\right\} e^{-\frac{r}{a_0}}$$

$$= \frac{1}{2a_0^3}\left\{\left(r-\frac{r^2}{2a_0}\right)\left(2-\frac{2r}{a_0}-\frac{r}{a_0}+\frac{r^2}{2a_0^2}\right)\right\} e^{-\frac{r}{a_0}}$$

$$= \frac{1}{2a_0^3}\left\{\left(r-\frac{r^2}{2a_0}\right)\left(2-\frac{3r}{a_0}+\frac{r^2}{2a_0^2}\right)\right\} e^{-\frac{r}{a_0}} \overset{!}{=} 0$$

$$\Rightarrow \quad r - r^2/2a_0 = 0 \quad \Rightarrow r_1 = 0, \quad r_2 = 2a_0$$

$$r^2 - 6a_0 r + 4a_0^2 \overset{!}{=} 0 \qquad r_{3/4} = a_0\left(3 \pm \sqrt{5}\right)$$

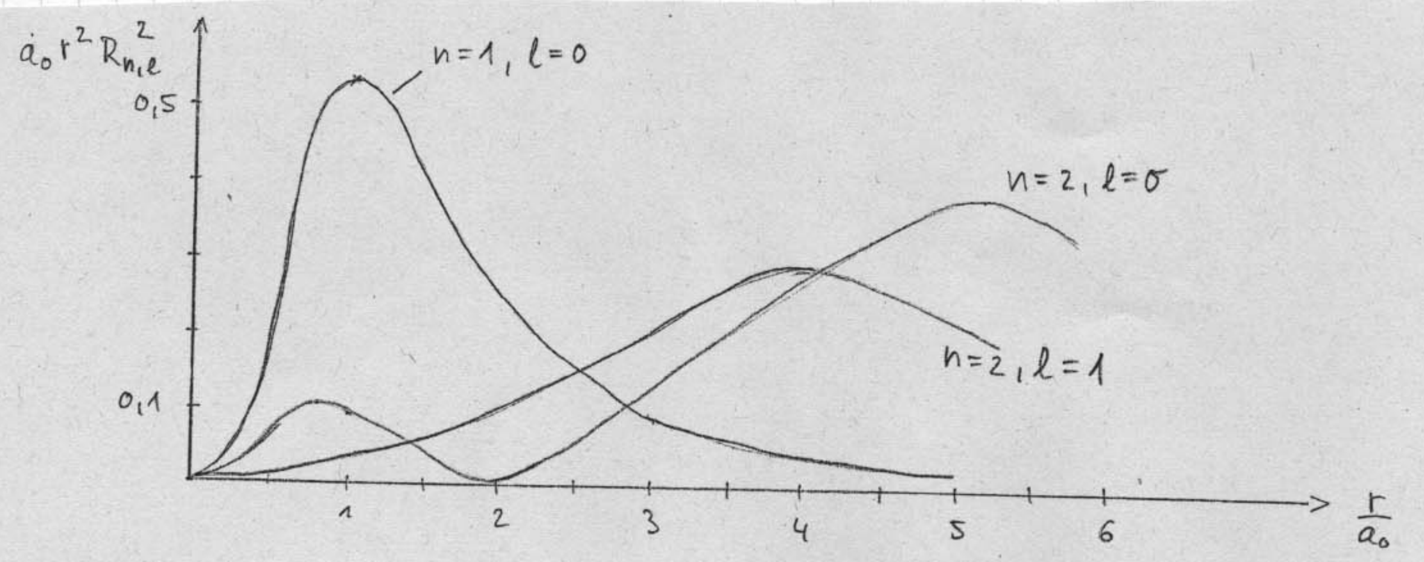
$n=2,\ l=1$

$$\frac{d}{dr}\left(r^2 R_{2,1}^2(r)\right) = \frac{d}{dr}\left(\frac{1}{6a_0^3}\frac{r^4}{4a_0^2} e^{-\frac{r}{a_0}}\right)$$

$$= \frac{1}{24a_0^5}\left(4r^3 - \frac{r^4}{a_0}\right) e^{-r/a_0}$$

$$\overset{!}{=} 0$$

$$\Rightarrow r_1 = 0 \qquad r_2 = 4a_0$$



Keine scharfen Werte im Gegensatz zu Bohr $\left(r_n = a_0 n^2\right)$

14) $1s: n=1, l=0, m=0$

$$\psi_{n,l,m} = R_{n,l}(r)\, Y_{l,m}(\vartheta, \varphi)$$

$$\langle \vec{r} \rangle = \iiint \vec{r}\, |\psi_{n,l,m}|^2\, dV \underline{\underline{= 0}}$$ für alle $\psi_{n,l,m}$,

da $|\psi|^2$ gerade und $\vec{r}(-x,-y,-z) = -\vec{r}(x,y,z)$ ungerade.

$$\langle r \rangle_{1,0} = \int_0^\infty \int_0^\pi \int_0^{2\pi} r \Big(\underbrace{\frac{1}{\sqrt{4\pi}}}_{Y_{0,0}} \cdot \underbrace{2\left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{r}{a_0}}}_{R_{1,0}} \Big)^2 r^2 \sin\theta \, dr\, d\theta\, d\varphi$$

$$= \frac{1}{4\pi}\, 4 \cdot \frac{1}{a_0^3} \int_0^\infty r^3 e^{-\frac{2r}{a_0}} dr \underbrace{\int_0^\pi \sin\theta\, d\theta \int_0^{2\pi} d\varphi}_{4\pi}$$

Klar, $Y_{l,m}$ sind normiert.

$$= \frac{4}{a_0^3} \underbrace{\int_0^\infty r^3 e^{-\frac{2r}{a_0}} dr}_{} = \underline{\underline{\frac{3}{2} a_0}}$$

mit $\int x^n e^{ax} dx = \frac{1}{a} x^n e^{ax} - \frac{n}{a} \int x^{n-1} e^{ax} dx$

und $\int x^2 e^{ax} dx$

$$= e^{ax}\left(\frac{x^2}{a} - \frac{2x}{a^2} + \frac{2}{a^3}\right)$$

$$\Rightarrow \int \ldots = \frac{3}{8} a_0^4$$

$\langle r^2 \rangle$: Betrachte nur Radialteil, da $Y_{l,m}$ bereits normiert (s.o.)

$$\langle r^2 \rangle_{1,0} = \int_0^\infty r^2 \left(2 \cdot \frac{1}{a_0^{3/2}} e^{-\frac{r}{a_0}} \right)^2 r^2 \, dr$$

$$= \frac{4}{a_0^3} \underbrace{\int_0^\infty r^4 e^{-\frac{2r}{a_0}} dr}_{\frac{3}{4} a_0^5} = \underline{\underline{3 a_0^2}}$$

15)

Tröpfchenmodell: $r_K \approx 1{,}3 \cdot 10^{-15} \, m \cdot \sqrt[3]{A}$

$r_H = 1{,}3 \; fm$ =

$r_{Na} = 3{,}7 \; fm$

Aufenthaltswahrscheinlichkeit $\quad \varrho = \iiint_{V_K} \psi^* \psi \, dV \underset{\substack{\uparrow \\ Y_{l,m} \text{ normiert (s.o.)}}}{=} \int_0^{r_K} r^2 R_{n,l}^2(r) \, dr$

Annahme: $R_{n,0}(r) = \text{const.} = R_{n,0}(0)$ für $r \leq r_K$, s-Elektronen: $l = 0$

$$\Rightarrow \varrho_K = R_{n,0}^2(0) \int_0^{r_K} r^2 \, dr = \frac{1}{3} r_K^3 R_{n,0}^2(0)$$

$R_{1,0}(0) = 2 \left(\frac{Z}{a_0} \right)^{3/2}$ $\qquad R_{1,0}^2(0) = 4 \left(\frac{Z}{a_0} \right)^3$

$R_{2,0}(0) = 2 \left(\frac{Z}{2a_0} \right)^{3/2}$ $\qquad R_{2,0}^2(0) = \frac{1}{2} \left(\frac{Z}{a_0} \right)^3$

$R_{3,0}(0) = 2 \left(\frac{Z}{3a_0} \right)^{3/2}$ $\qquad R_{3,0}^2(0) = \frac{4}{27} \left(\frac{Z}{a_0} \right)^3$ $\qquad$ mit $Z = 1$ für H, $Z = 11$ für Na

	1s	2s	3s
ϱ_H	$1{,}98 \cdot 10^{-14}$	$2{,}47 \cdot 10^{-15}$	$7{,}33 \cdot 10^{-16}$
$\varrho_{Na^{10+}}$	$6{,}07 \cdot 10^{-10}$	$7{,}59 \cdot 10^{-11}$	$2{,}25 \cdot 10^{-11}$