Blatt 4

Aufgabe 13

a)
$$\langle \vec{L}^2 \rangle = l(l+1)\hbar^2 \quad \text{mit} \quad l = 0, 1, 2, \dots, n-1$$
$$\langle L_z \rangle = m\hbar \quad \text{mit} \quad m = 0, \pm 1, \pm 2, \dots, \pm l$$

$n = 5$

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

$n = 6$

$l = 0 \qquad m = 0$
$\vdots$ (analog $n = 5$)
$l = 5 \qquad m = 0, \pm 1, \pm 2, \pm 3, \pm 4, \pm 5$

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

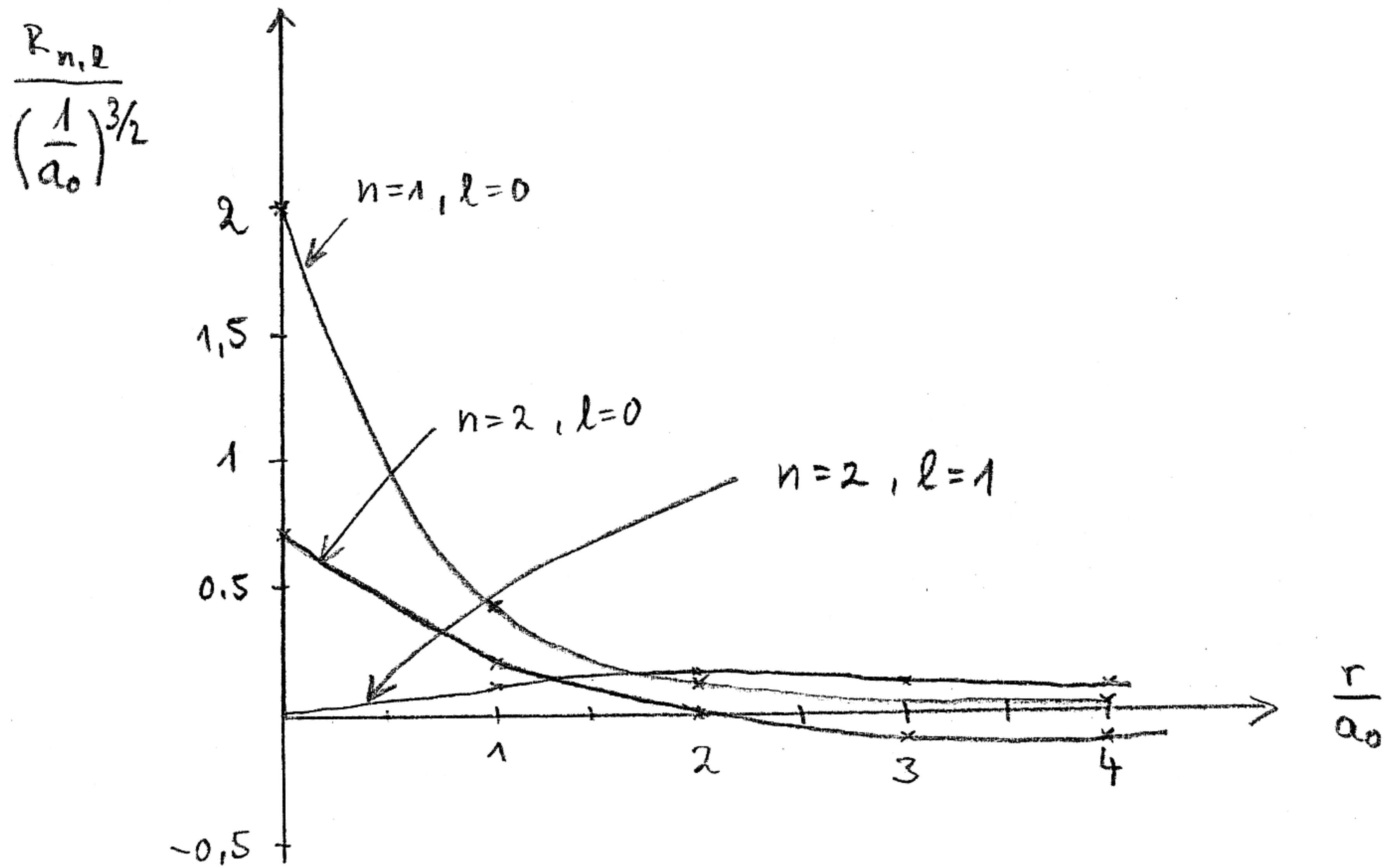
$\Rightarrow$ keine Nullstelle !

$n = 2$, $l = 0$:
$$R_{2,0} = 2\left(\frac{1}{2a_0}\right)^{\frac{3}{2}}\left(1 - \frac{r}{2a_0}\right)\cdot e^{-\frac{r}{2a_0}}$$

$\Rightarrow$ Nullstelle : $r_0 = 2a_0$

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

$\Rightarrow$ Nullstelle $r_0 = 0$


$\frac{R_{n,l}}{\left(\frac{1}{a_0}\right)^{3/2}}$
2
1,5
1
0,5
-0,5
$n=1, l=0$
$n=2, l=0$
$n=2, l=1$
1
2
3
4
$\frac{r}{a_0}$

c) $\int_r^{r+\Delta r} r^2 R_{n,l}^2 (r')\,dr'$ Beschreibt die Aufenthaltswahrscheinlichkeit des Elektrons in einer Kugelschale vom Radius r und der Dicke Δr.

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

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

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

$$= \frac{4}{a_0^3}\left[r^2\left(-\frac{a_0}{2}\right)e^{-\frac{2r}{a_0}}\right]_0^\infty - \frac{4}{a_0^3}\int_0^\infty 2r\left(-\frac{a_0}{2}\right)e^{-\frac{2r}{a_0}}\,dr$$

$$= \frac{4}{a_0^3}\left\{\left[r^2\left(-\frac{a_0}{2}\right)e^{-\frac{2r}{a_0}}\right]_0^\infty - 2\left(\left[r\left(-\frac{a_0}{2}\right)^2 e^{-\frac{2r}{a_0}}\right]_0^\infty - \int_0^\infty \left(-\frac{a_0}{2}\right)^2 e^{-\frac{2r}{a_0}}\,dr\right)\right\}$$

$$= \frac{4}{a_0^3}\left\{0 - 0 + 2\left[\left(-\frac{a_0}{2}\right)^3 e^{-\frac{2r}{a_0}}\right]_0^\infty\right\}$$

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

Normierung: Das Elektron ist irgendwo.

d) $\underline{n=1}$: $r^2 R_{1,0}^2 = \frac{4}{a_0^3} r^2 e^{-\frac{2r}{a_0}}$

$$\frac{d}{dr}\left(r^2 R_{1,0}^2\right) = \frac{4}{a_0^3}\left(2r e^{-\frac{2r}{a_0}} - \frac{2r^2}{a_0} e^{-\frac{2r}{a_0}}\right) \overset{!}{=} 0$$

$\Rightarrow$ gilt für $r_1 = 0$ und $r_2 = a_0$

$\underline{n = 2,\ l = 0:}$

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

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

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

$$\stackrel{!}{=} 0$$

$$\Rightarrow \quad r-\frac{r^2}{2a_0} = 0 \quad \vee \quad r^2-6a_0 r+4a_0^2 = 0$$

$$\Leftrightarrow \quad r_1 = 0 \quad \vee \quad r_2 = 2a_0 \quad \vee \quad r_3 = a_0(3+\sqrt{5}) \quad \vee \quad r_4 = a_0(3-\sqrt{5})$$

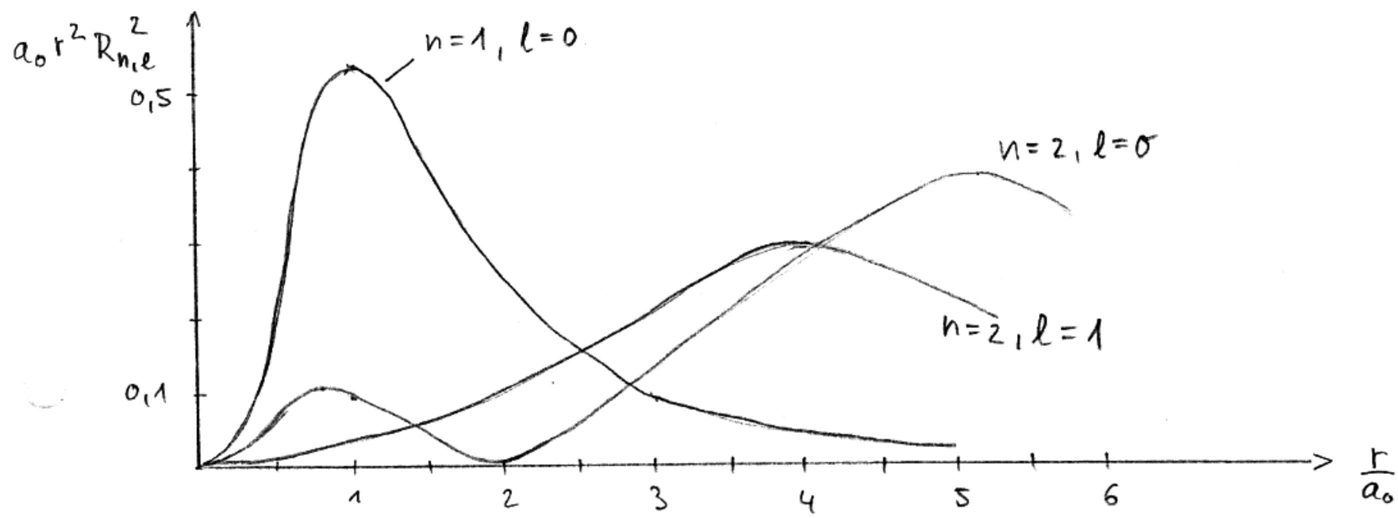
$\underline{n = 2,\ l = 1:}$

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

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

$$\stackrel{!}{=} 0$$

$$\Rightarrow \quad r_1 = 0 \quad \vee \quad r = 4a_0$$



Unterschied zu Bohr ($r_n = a_0 n^2$): keine diskreten / scharfen Werte, aber für jeweils "l" höchste Wahrscheinlichkeit $r^2 R^2 dr$ bei $n^2 a_0$

e) Kernradius $r_h = 4{,}7 \cdot 10^{-15}\,m$

Aufenthaltswahrscheinlichkeit

$$\rho = \iiint_{V_h} \psi^* \psi \, dV \underset{\uparrow}{=} \int_0^{r_h} r^2 R_{n,l}^2(r)\, dr$$

Normierte Kugelflächenfunktionen (s. Vorlesung)

Annahme: $R_{n,0}(r) = \text{const.} = R_{n,0}(0)$ für $r \leq r_h$

s-Elektronen: $l = 0$

$$\Rightarrow \rho_{n0} = R_{n,0}^2(0) \int_0^{r_h} r^2\, dr = \frac{1}{3} r_h^3 \, R_{n,0}^2$$

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

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

$$R_{3,0}(0) = 2\left(\frac{Z}{3a_0}\right)^{\frac{3}{2}} \quad ; \quad R_{3,0}^2(0) = \frac{4}{27}\left(\frac{Z}{a_0}\right)^3$$

<u>1s:</u> $\rho_{10} = \frac{1}{3} r_h^3 \cdot 4\left(\frac{Z}{a_0}\right)^3 = \frac{4}{3} \cdot \underbrace{\left(\frac{r_h Z}{a_0}\right)}_{\approx 2 \cdot 10^{-3}}{}^3 \approx 1{,}067 \cdot 10^{-8}$

<u>2s:</u> $\rho_{20} = \frac{1}{3} r_h^3 \cdot \frac{1}{2}\left(\frac{Z}{a_0}\right)^3 = \frac{1}{6}\left(\frac{r_h Z}{a_0}\right)^3 \approx 1{,}333 \cdot 10^{-9}$

<u>3s:</u> $\rho_{30} = \frac{1}{3} r_h^3 \frac{4}{27}\left(\frac{Z}{a_0}\right)^3 = \frac{4}{81}\left(\frac{r_h Z}{a_0}\right)^3 \approx 3{,}951 \cdot 10^{-10}$

f) $n = 3 \; ; \; l = 2$

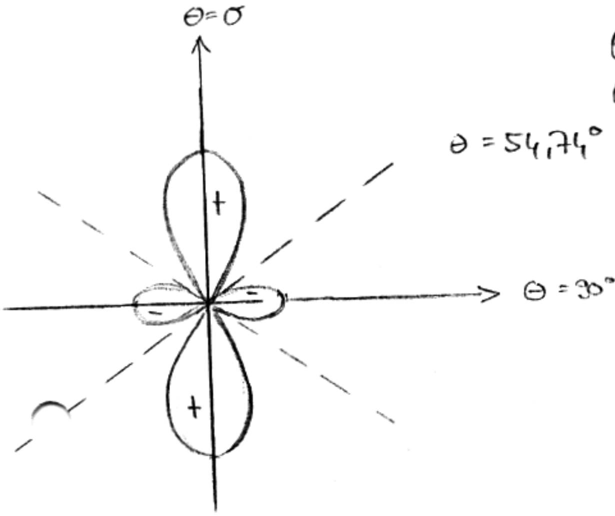
Winkelabhängigkeit: $Y_{l,m}(\theta, \varphi)$; $l = 2, \; \varphi = 0$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}} \, (3\cos^2\theta - 1)$$

$\theta = 0°$: $3\cos^2\theta - 1 = 2$

$\theta = 54{,}74°$: $3\cos^2\theta - 1 = 0$

$\theta = 90°$: $3\cos^2\theta - 1 = -1$



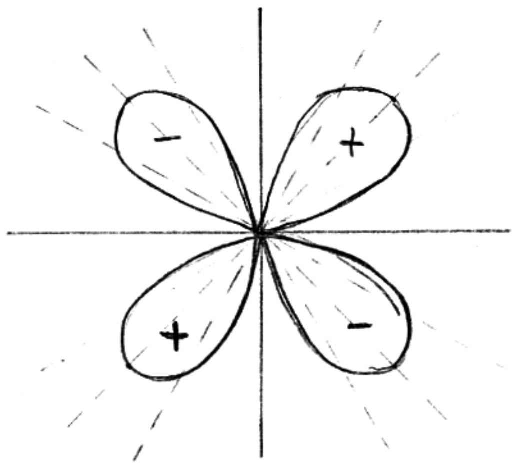
$$Y_{2,\pm 1} = \sqrt{\frac{15}{8\pi}} \cos\theta \sin\theta \, e^{\mp i\varphi}$$

$\theta = 0°$: $\cos\theta \sin\theta = 0$

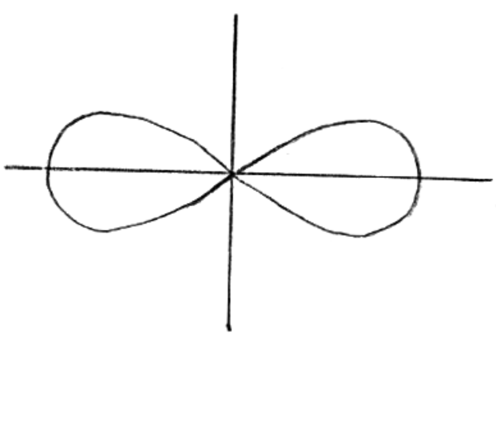
$\theta = 90°$: $\cos\theta \sin\theta = 0$

$\theta = 45°$: $\cos\theta \sin\theta = \frac{1}{2}$

$\theta = 30°$: $\cos\theta \sin\theta = \frac{\sqrt{3}}{4} \approx 0{,}43$



$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta \, e^{\pm i 2\varphi}$$



g) $L_z \hat{=} \frac{\hbar}{i} \partial_\varphi$

$$L_z \psi = \frac{\hbar}{i} \partial_\varphi \left\{ A r^2 e^{-\frac{r}{3a_0}} \sin\theta \cos\theta \, e^{i\varphi} \right\}$$

$$= \frac{\hbar}{i} \, i \, \psi = \hbar \psi \quad \Rightarrow \quad \underline{\underline{m = +1}}$$

$\ulcorner$ Denn: $\langle L_z \rangle = \iiint \psi^* L_z \psi \, dV = m \hbar$

$$= \iiint \psi^* h \psi \, dV = \hbar \iiint \psi^* \psi \, dV = h \lrcorner$$

$$\langle \vec{L}^2 \rangle = \ell(\ell+1) \hbar^2$$ (nicht $\vec{L}\psi \rightarrow$ Unschärferelation)

$$\vec{L}^2 \psi = -\hbar^2 \Big(\underbrace{\frac{1}{\sin\theta} \partial\theta (\sin\theta \partial_\theta)}_{1. \text{ Teil}} + \underbrace{\frac{1}{\sin^2\theta} \partial^2_\varphi}_{2. \text{ Teil}} \Big) \psi$$

1. Teil: $\frac{1}{\sin\theta} \partial_\theta (\sin\theta \, \partial_\theta) \sin\theta \cos\theta$

$$= \frac{1}{\sin\theta} \partial_\theta \quad \sin\theta (\cos^2\theta - \sin^2\theta)$$
$$= \frac{\cos\theta}{\sin\theta} (\cos^2\theta - \sin^2\theta) - 4 \cos\theta \sin\theta$$

2. Teil: $\frac{1}{\sin^2\theta} \partial^2_\varphi \sin\theta \cos\theta \, e^{i\varphi} = - \frac{\cos\theta}{\sin\theta} \, e^{i\varphi}$

also insgesamt: $$\vec{L}^2 \psi = A r^2 e^{-\frac{r}{3a_0}} \left[\frac{\cos\theta}{\sin\theta} (1 - 2 \sin^2\theta - 4 \cos\theta \sin\theta - \frac{\cos\theta}{\sin\theta} \right] e^{i\varphi} (-\hbar)^2$$
$$= 6 \hbar^2 \psi \overset{!}{=} \ell(\ell+1) \hbar^2 \psi$$
$$\Rightarrow \underline{\underline{\ell = 2}}$$

Hauptquantenzahl: $e^{-\frac{r}{3a_0}} \Rightarrow \underline{\underline{n = 3}}$

h) 1s Zustand: $n=1$; $l=0$, $m=0$

$$\langle \vec{r} \rangle = \iiint \psi^*_{n,l,m} \, \vec{r} \, \psi_{n,l,m} \, dV = \iiint |\psi_{n,l,m}|^2 \vec{r} \, dV$$

$$|\psi_{n,l,m}(\vec{r})|^2 = |\psi_{n,l,m}(-\vec{r})|^2 \quad ; \text{d. h gerade}$$

$$\vec{r}(-x,-y,-z) = -\vec{r}(x,y,z) \quad ; \text{ungerade}$$

$$\Rightarrow \langle \vec{r} \rangle = 0$$

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

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

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

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

und $\int x^2 e^{ax} dx = e^{ax} \left[\frac{x^2}{a} - \frac{2x}{a^2} + \frac{2}{a^3} \right]$

$$= \frac{4}{a_0^3} \cdot \frac{3}{8} a_0^4 = \underline{\underline{\frac{3}{2} a_0}}$$

$\langle r^2 \rangle$: Betrachte nur Radialteil, da $Y_{l,m}$ normiert

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

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