Problem 4.55

(a) Use the recursion formula (Equation 4.76) to confirm that when $\ell = n-1$ the radial wave function takes the form

$$R_{n(n-1)} = N_n r^{n-1} e^{-r/na},$$

and determine the normalization constant N_n by direct integration.

(b) Calculate $\langle r \rangle$ and $\langle r^2 \rangle$ for states of the form $\psi_{n(n-1)m}$.

(c) Show that the "uncertainty" in r (σ_r) is $\langle r \rangle / \sqrt{2n+1}$ for such states. Note that the fractional spread in r decreases, with increasing n (in this sense the system "begins to look classical," with identifiable circular "orbits," for large n). Sketch the radial wave functions for several values of n, to illustrate this point.

Solution

Part (a)

Equation 4.76 is on page 147.

$$c_{j+1} = \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)} c_j \tag{4.76}$$

It's the recursion relation for the coefficients in the radial wave function.

$$R_{n\ell}(r) = \frac{1}{r}\rho^{\ell+1}e^{-\rho}v(\rho) \tag{4.75}$$

$$= \frac{1}{r}\rho^{\ell+1}e^{-\rho}\sum_{j=0}^{\infty} c_j \rho^j$$

$$= \frac{1}{r}\left(\frac{r}{na_0}\right)^{\ell+1} e^{-r/(na_0)} \sum_{j=0}^{\infty} c_j \left(\frac{r}{na_0}\right)^j$$

Set $\ell = n-1$ in the function.

$$R_{n(n-1)}(r) = \frac{1}{r}\left(\frac{r}{na_0}\right)^{(n-1)+1} e^{-r/(na_0)} \sum_{j=0}^{\infty} c_j \left(\frac{r}{na_0}\right)^j$$

$$= \frac{1}{r}\left(\frac{r}{na_0}\right)^{n} e^{-r/(na_0)} \sum_{j=0}^{\infty} c_j \left(\frac{r}{na_0}\right)^j$$

$$= \frac{1}{n^n a_0^n} r^{n-1} e^{-r/(na_0)} \sum_{j=0}^{\infty} c_j \left(\frac{r}{na_0}\right)^j$$

Set $\ell = n - 1$ in the recursion relation.

$$\begin{aligned} c_{j+1} &= \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)}c_j \\ &= \frac{2[j+(n-1)+1-n]}{(j+1)[j+2(n-1)+2]}c_j \\ &= \frac{2j}{(j+1)(j+2n)}c_j \end{aligned}$$

Solve for c_j by writing out the first few terms until a pattern becomes apparent.

$$\begin{aligned} c_1 &= \frac{2(0)}{(0+1)(0+2n)}c_0 = 0 \\ c_2 &= \frac{2(1)}{(1+1)(1+2n)}c_1 = 0 \\ c_3 &= \frac{2(2)}{(2+1)(2+2n)}c_2 = 0 \\ &\vdots \\ c_j &= 0, \quad j \neq 0 \end{aligned}$$

As a result, the infinite series in the radial wave function terminates right away.

$$\begin{aligned} R_{n(n-1)}(r) &= \frac{1}{n^n a_0^n} r^{n-1} e^{-r/(na_0)} \sum_{j=0}^{\infty} c_j \left(\frac{r}{na_0}\right)^j \\ &= \frac{1}{n^n a_0^n} r^{n-1} e^{-r/(na_0)} \left[\underbrace{c_0\left(\frac{r}{na_0}\right)^0}_{=c_0} + \underbrace{c_1\left(\frac{r}{na_0}\right)^1}_{=0} + \underbrace{c_2\left(\frac{r}{na_0}\right)^2}_{=0} + \cdots\right] \\ &= \left(\frac{c_0}{n^n a_0^n}\right) r^{n-1} e^{-r/(na_0)} \\ &= N_n r^{n-1} e^{-r/(na_0)} \end{aligned}$$

N_n is a normalization constant.

The normalization of the stationary states requires that

$$1 = \iiint_{\text{all space}} |\Psi_{n\ell m}(r,\theta,\phi,t)|^2\,d\mathcal{V} = \iiint_{\text{all space}} |R_{n\ell}(r)Y_\ell^m(\theta,\phi)T_n(t)|^2\,d\mathcal{V}$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^\infty |R_{n\ell}(r)|^2 |Y_\ell^m(\theta,\phi)|^2 |e^{-iE_nt/\hbar}|^2\,(r^2\sin\theta\,dr\,d\phi\,d\theta)$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^\infty |R_{n\ell}(r)|^2 |Y_\ell^m(\theta,\phi)|^2\,(r^2\sin\theta\,dr\,d\phi\,d\theta)$$

$$= \underbrace{\left[\int_0^\infty r^2 |R_{n\ell}(r)|^2\,dr\right]}_{=1} \underbrace{\left[\int_0^\pi \int_0^{2\pi} |Y_\ell^m(\theta,\phi)|^2 \sin\theta\,d\phi\,d\theta\right]}_{=1},$$

which means

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

$$= \int_0^\infty r^2 \left[N_n^2 r^{2(n-1)} e^{-2r/(na_0)}\right] dr$$

$$= N_n^2 \int_0^\infty r^{2n} e^{-2r/(na_0)}\,dr.$$

Use tabulated integration-by-parts to evaluate the integral.

	$\frac{d}{dr}$	$\int dr$
$+$	r^{2n}	$e^{-2r/(na_0)}$
$-$	$(2n)r^{2n-1}$	$\left(-\frac{na_0}{2}\right)e^{-2r/(na_0)}$
$+$	$(2n)(2n-1)r^{2n-2}$	$\left(\frac{n^2a_0^2}{4}\right)e^{-2r/(na_0)}$
$-$	$(2n)(2n-1)(2n-2)r^{2n-3}$	$\left(-\frac{n^3a_0^3}{8}\right)e^{-2r/(na_0)}$
	$\cdots$	$\cdots$
$+$	$(2n)!\,r^0$	$(-1)^{2n}\left(\frac{n^{2n}a_0^{2n}}{2^{2n}}\right)e^{-2r/(na_0)}$
$-$	0	$-\left(\frac{n^{2n+1}a_0^{2n+1}}{2^{2n+1}}\right)e^{-2r/(na_0)}$

Consequently,

$$1 = N_n^2 \Bigg[\overbrace{\left(-\frac{na_0}{2}\right) r^{2n} e^{-2r/(na_0)}\Big|_0^\infty}^{=0} - \overbrace{(2n)\left(\frac{n^2a_0^2}{4}\right) r^{2n-1} e^{-2r/(na_0)}\Big|_0^\infty}^{=0} - \overbrace{(2n)(2n-1)\left(\frac{n^3a_0^3}{8}\right) r^{2n-2} e^{-2r/(na_0)}\Big|_0^\infty}^{=0}$$

$$- \cdots$$

$$- (2n)!\frac{n^{2n+1}a_0^{2n+1}}{2^{2n+1}} r^0 e^{-2r/(na_0)}\Big|_0^\infty \Bigg]$$

$$= N_n^2 (2n)!\frac{n^{2n+1}a_0^{2n+1}}{2^{2n+1}}.$$

Solve for N_n^2.

$$N_n^2 = \left(\frac{2^n}{n^n a_0^n}\right)^2 \frac{2}{na_0(2n)!}$$

Take the square root of both sides.

$$\boxed{N_n = \frac{2^n}{n^n a_0^n}\sqrt{\frac{2}{na_0(2n)!}}}$$

Part (b)

Calculate $\langle r \rangle$ for the stationary state $\Psi_{n(n-1)m}$.

$$\langle r \rangle = \frac{\langle \Psi_{n(n-1)m} \,|\, r \,|\, \Psi_{n(n-1)m} \rangle}{\langle \Psi_{n(n-1)m} \,|\, \Psi_{n(n-1)m} \rangle} = \frac{\displaystyle\iiint_{\text{all space}} \Psi^*_{n(n-1)m} r \Psi_{n(n-1)m}\, d\mathcal{V}}{\displaystyle\iiint_{\text{all space}} \Psi^*_{n(n-1)m} \Psi_{n(n-1)m}\, d\mathcal{V}}$$

$$= \frac{\displaystyle\iiint_{\text{all space}} \left[R_{n(n-1)}(r) Y_{n-1}^m(\theta,\phi) e^{iE_nt/\hbar}\right]^* r \left[R_{n(n-1)}(r) Y_{n-1}^m(\theta,\phi) e^{iE_nt/\hbar}\right] d\mathcal{V}}{1}$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^\infty r|R_{n(n-1)}(r)|^2 |Y_{n-1}^m(\theta,\phi)|^2 (r^2 \sin\theta\, dr\, d\phi\, d\theta)$$

$$= \int_0^\infty r^3 |R_{n(n-1)}(r)|^2\, dr \underbrace{\left[\int_0^\pi \int_0^{2\pi} |Y_{n-1}^m(\theta,\phi)|^2 \sin\theta\, d\phi\, d\theta\right]}_{=1}$$

$$= N_n^2 \int_0^\infty r^{2n+1} e^{-2r/(na_0)}\, dr$$

Use tabulated integration-by-parts again to evaluate the integral.

	$\frac{d}{dr}$	$\int dr$
$+$	r^{2n+1}	$e^{-2r/(na_0)}$
$-$	$(2n+1)r^{2n}$	$\left(-\frac{na_0}{2}\right)e^{-2r/(na_0)}$
$+$	$(2n+1)(2n)r^{2n-1}$	$\left(\frac{n^2a_0^2}{4}\right)e^{-2r/(na_0)}$
$-$	$(2n+1)(2n)(2n-1)r^{2n-2}$	$\left(-\frac{n^3a_0^3}{8}\right)e^{-2r/(na_0)}$
	$\cdots$	$\cdots$
$-$	$(2n+1)!\,r^0$	$(-1)^{2n+1}\left(\frac{n^{2n+1}a_0^{2n+1}}{2^{2n+1}}\right)e^{-\frac{2r}{na_0}}$
$+$	0	$\left(\frac{n^{2n+2}a_0^{2n+2}}{2^{2n+2}}\right)e^{-2r/(na_0)}$

Therefore,

$$\langle r\rangle = N_n^2\left[\overbrace{\left(-\frac{na_0}{2}\right)r^{2n+1}e^{-2r/(na_0)}\Big|_0^\infty}^{=0} - \overbrace{(2n+1)\left(\frac{n^2a_0^2}{4}\right)r^{2n}e^{-2r/(na_0)}\Big|_0^\infty}^{=0}\right.$$

$$- \overbrace{(2n+1)(2n)\left(\frac{n^3a_0^3}{8}\right)r^{2n-1}e^{-2r/(na_0)}\Big|_0^\infty}^{=0} - \cdots$$

$$\left. - (2n+1)!\frac{n^{2n+2}a_0^{2n+2}}{2^{2n+2}}r^0e^{-2r/(na_0)}\Big|_0^\infty\right]$$

$$= N_n^2(2n+1)!\frac{n^{2n+2}a_0^{2n+2}}{2^{2n+2}}$$

$$= \left(\frac{2^n}{n^na_0^n}\right)^2\frac{2}{na_0(2n)!}(2n+1)!\frac{n^{2n+2}a_0^{2n+2}}{2^{2n+2}}$$

$$= \frac{2}{na_0}(2n+1)\frac{n^2a_0^2}{2^2}$$

$$\boxed{\langle r\rangle = \frac{na_0}{2}(2n+1).}$$

Calculate $\langle r^2 \rangle$ for the stationary state $\Psi_{n(n-1)m}$.

$$\langle r^2 \rangle = \frac{\langle \Psi_{n(n-1)m} \,|\, r^2 \,|\, \Psi_{n(n-1)m} \rangle}{\langle \Psi_{n(n-1)m} \,|\, \Psi_{n(n-1)m} \rangle} = \frac{\displaystyle\iiint_{\text{all space}} \Psi^*_{n(n-1)m} r^2 \Psi_{n(n-1)m} \, d\mathcal{V}}{\displaystyle\iiint_{\text{all space}} \Psi^*_{n(n-1)m} \Psi_{n(n-1)m} \, d\mathcal{V}}$$

$$= \frac{\displaystyle\iiint_{\text{all space}} \left[R_{n(n-1)}(r) Y^m_{n-1}(\theta, \phi) e^{iE_n t/\hbar} \right]^* r^2 \left[R_{n(n-1)}(r) Y^m_{n-1}(\theta, \phi) e^{iE_n t/\hbar} \right] d\mathcal{V}}{1}$$

$$= \int_0^\pi \int_0^{2\pi} \int_0^\infty r^2 |R_{n(n-1)}(r)|^2 |Y^m_{n-1}(\theta, \phi)|^2 (r^2 \sin\theta \, dr \, d\phi \, d\theta)$$

$$= \int_0^\infty r^4 |R_{n(n-1)}(r)|^2 \, dr \underbrace{\left[\int_0^\pi \int_0^{2\pi} |Y^m_{n-1}(\theta, \phi)|^2 \sin\theta \, d\phi \, d\theta \right]}_{=\,1}$$

$$= \int_0^\infty r^4 \left[N_n^2 r^{2(n-1)} e^{-2r/(na_0)} \right] dr$$

$$= N_n^2 \int_0^\infty r^{2n+2} e^{-2r/(na_0)} \, dr$$

Use tabulated integration-by-parts again to evaluate the integral.

	$\frac{d}{dr}$	$\int dr$
$+$	r^{2n+2}	$e^{-2r/(na_0)}$
$-$	$(2n+2)r^{2n+1}$	$\left(-\frac{na_0}{2}\right)e^{-2r/(na_0)}$
$+$	$(2n+2)(2n+1)r^{2n}$	$\left(\frac{n^2a_0^2}{4}\right)e^{-2r/(na_0)}$
$-$	$(2n+2)(2n+1)(2n)r^{2n-1}$	$\left(-\frac{n^3a_0^3}{8}\right)e^{-2r/(na_0)}$
	$\cdots$	$\cdots$
$+$	$(2n+2)!\,r^0$	$(-1)^{2n+2}\left(\frac{n^{2n+2}a_0^{2n+2}}{2^{2n+2}}\right)e^{-\frac{2r}{na_0}}$
$-$	0	$-\left(\frac{n^{2n+3}a_0^{2n+3}}{2^{2n+3}}\right)e^{-2r/(na_0)}$

Therefore,

$$\langle r^2\rangle = N_n^2\Bigg[\overbrace{\left(-\frac{na_0}{2}\right)r^{2n+2}e^{-2r/(na_0)}\Big|_0^\infty}^{=0} - \overbrace{(2n+2)\left(\frac{n^2a_0^2}{4}\right)r^{2n+1}e^{-2r/(na_0)}\Big|_0^\infty}^{=0}$$

$$- \overbrace{(2n+2)(2n+1)\left(\frac{n^3a_0^3}{8}\right)r^{2n}e^{-2r/(na_0)}\Big|_0^\infty}^{=0} - \cdots$$

$$- (2n+2)!\frac{n^{2n+3}a_0^{2n+3}}{2^{2n+3}}r^0e^{-2r/(na_0)}\Big|_0^\infty\Bigg]$$

$$= N_n^2(2n+2)!\frac{n^{2n+3}a_0^{2n+3}}{2^{2n+3}}$$

$$= \left(\frac{2^n}{n^na_0^n}\right)^2\frac{2}{na_0(2n)!}(2n+2)!\frac{n^{2n+3}a_0^{2n+3}}{2^{2n+3}}$$

$$= \frac{2}{na_0}(2n+1)(2n+2)\frac{n^3a_0^3}{2^3}$$

$$\boxed{\langle r^2\rangle = \frac{n^2a_0^2}{2}(2n+1)(n+1).}$$

Part (c)

The uncertainty in r for the stationary state $\Psi_{n(n-1)m}$ is therefore

$$\begin{aligned}
\sigma_r &= \sqrt{\langle r^2\rangle - \langle r\rangle^2} \\
&= \sqrt{\frac{n^2a_0^2}{2}(2n+1)(n+1) - \left[\frac{na_0}{2}(2n+1)\right]^2} \\
&= \sqrt{\frac{n^2a_0^2}{4}(2n+1)(2n+2) - \frac{n^2a_0^2}{4}(2n+1)^2} \\
&= \sqrt{\frac{n^2a_0^2}{4}(2n+1)^2\left(\frac{2n+2}{2n+1} - 1\right)} \\
&= \frac{na_0}{2}(2n+1)\sqrt{\frac{2n+2}{2n+1} - 1} \\
&= \langle r\rangle\sqrt{\frac{(2n+2)-(2n+1)}{2n+1}} \\
&= \langle r\rangle\sqrt{\frac{1}{2n+1}}
\end{aligned}$$

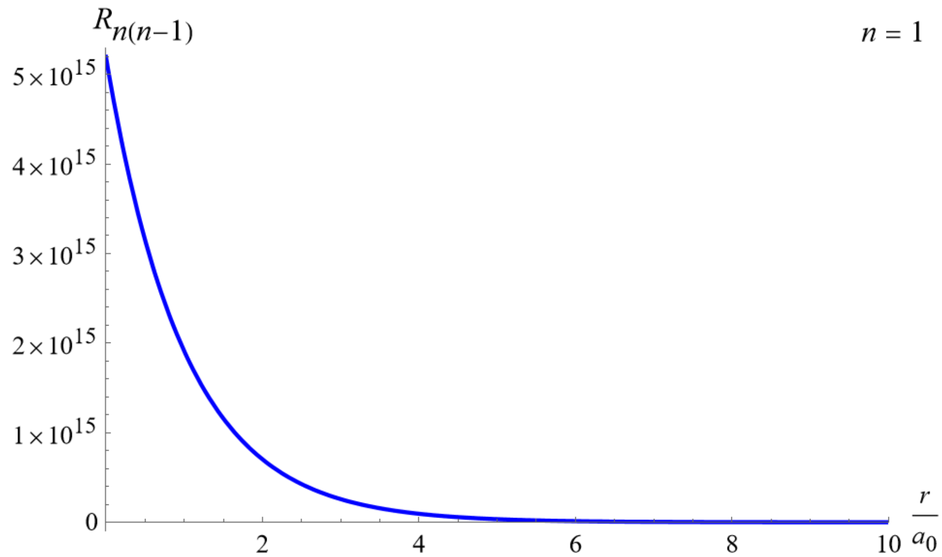
$$\boxed{\sigma_r = \frac{\langle r\rangle}{\sqrt{2n+1}}.}$$

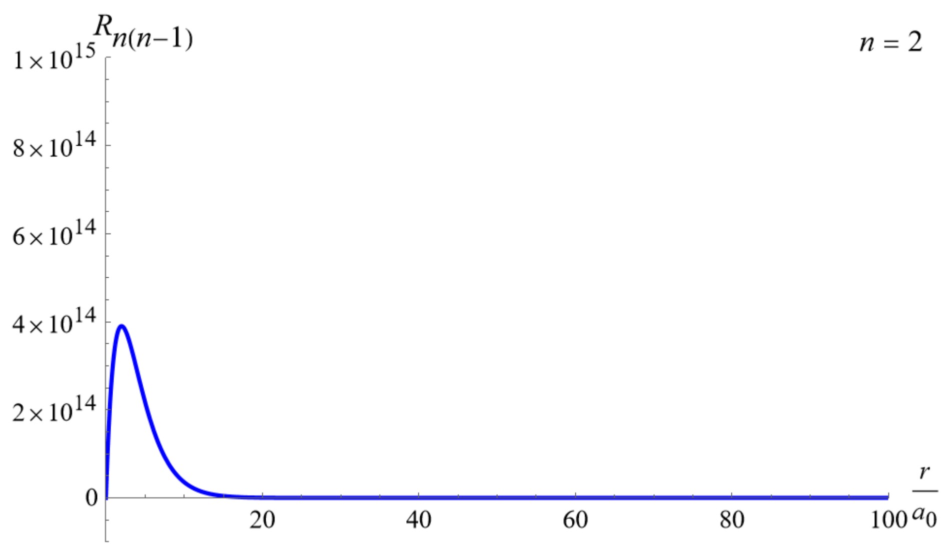
The radial wave functions with $\ell = n-1$ are given by

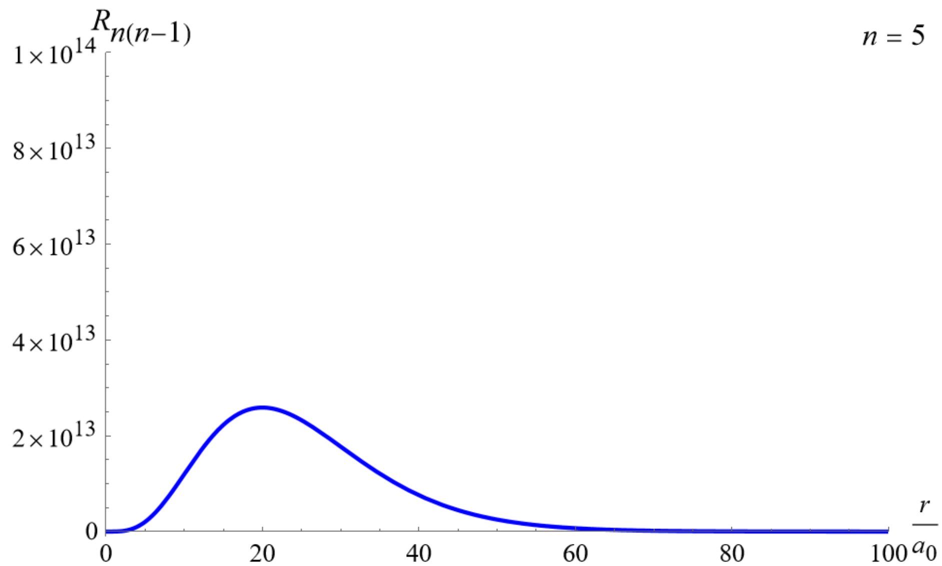
$$\begin{aligned}
R_{n(n-1)}(r) &= N_n r^{n-1} e^{-r/(na_0)} \\
&= \frac{2^n}{n^n a_0^n}\sqrt{\frac{2}{na_0(2n)!}}\, r^{n-1}e^{-r/(na_0)}, \quad n = 1, 2, 3, \ldots \\
&= \frac{2^n}{n^n a_0}\sqrt{\frac{2}{na_0(2n)!}}\left(\frac{r}{a_0}\right)^{n-1}\exp\left[-\frac{1}{n}\left(\frac{r}{a_0}\right)\right],
\end{aligned}$$

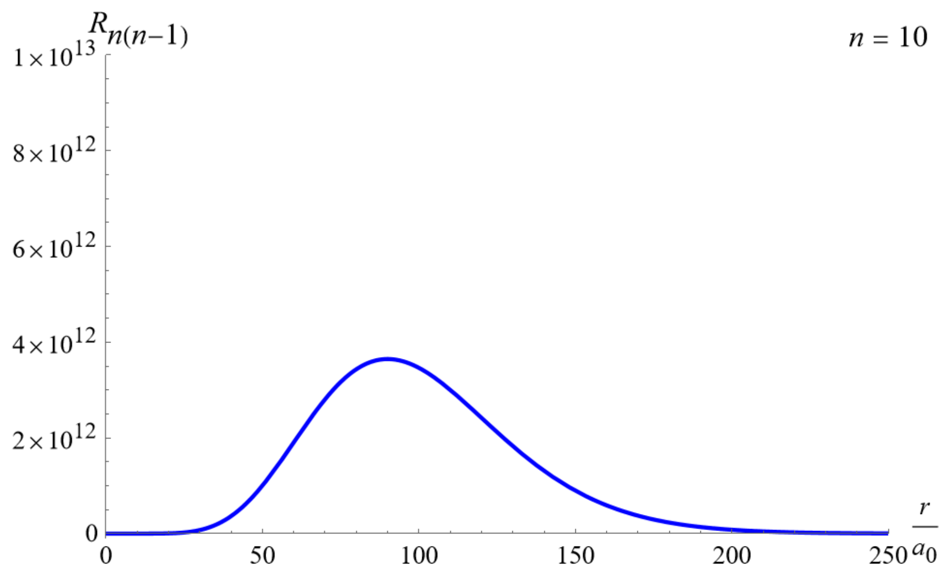
where $a_0 \approx 5.29\times10^{-11}$ m is the Bohr radius.

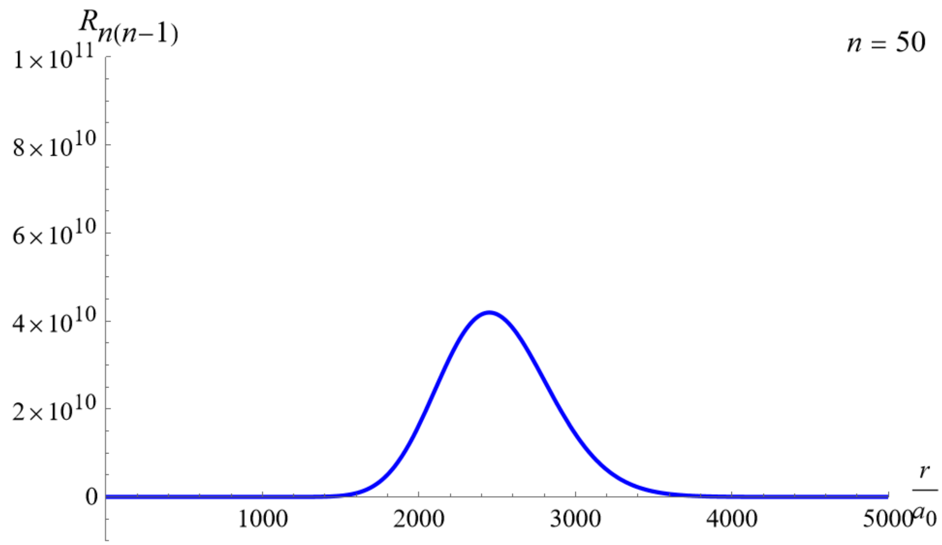
They're graphed below for several values of n.






$R_{n(n-1)}$
$n = 5$
1×10^{14}
8×10^{13}
6×10^{13}
4×10^{13}
2×10^{13}
0
0
20
40
60
80
100
$\frac{r}{a_0}$


$R_{n(n-1)}$
$n = 10$
1×10^{13}
8×10^{12}
6×10^{12}
4×10^{12}
2×10^{12}
0
0
50
100
150
200
250
$\frac{r}{a_0}$


$R_{n(n-1)}$
$n = 50$
1×10^{11}
8×10^{10}
6×10^{10}
4×10^{10}
2×10^{10}
0
1000
2000
3000
4000
5000
$\frac{r}{a_0}$