```
> restart; interface(displayprecision = 3) :
> with(plots) :
```

Using Maple's Associated Laguerre Polynomial Function

```
> MALa := proc(n, a, x) simplify((n + a)! LaguerreL(n, a, x)); end proc:
```

Hydrogen Atom Radial Function

```
> R := (n, l) → (2/(a·n))^(3/2) · sqrt((n − l − 1)!/(2·n·((n + l)!)^3)) · e^(−r/(a·n)) · (2·r/(n·a))^l · MALa(n − l − 1, 2·l + 1, 2·r/(a·n)) :
```

Hydrogen Atom Radial Probability

```
> P := (n, l) → r^2 · (abs(R(n, l)))^2 :
```

Graph of the Radial Function $R(n, l)$

```
> graph := proc(n, l)
    local g, h, v, tk, N;
    global a;
    a := 0.529; v := 1; h := 1;
    N := 7·n; tk := 10;
    if n = 4 then tk := 15 end if;
    g := plot(R(n, l), r = 0..N,
        color = red, axis[1] = [gridlines = [14·v, linestyle = solid]],
        thickness = 2, axis[2] = [gridlines = [12·h, linestyle = solid]],
        tickmarks = [tk, 3]) :
    a := 'a';
    display([g]);
  end proc:
```

Graph of the Radial Distribution $R^2(n, l)\ r^2$

```
> graphP := proc(n, l)
    local g, h, v, tk, N;
    global a;
    a := 0.529; h := 1; v := 1;
    N := 7·n; tk := 10;
    if n = 4 then tk := 15 end if;
    g := plot(P(n, l), r = 0..N,
        color = red, axis[1] = [gridlines = [14·v, linestyle = solid]],
        thickness = 2, axis[2] = [gridlines = [12·h, linestyle = solid]],
        tickmarks = [tk, 3]) :
    a := 'a';
    display([g]);
  end proc:
```

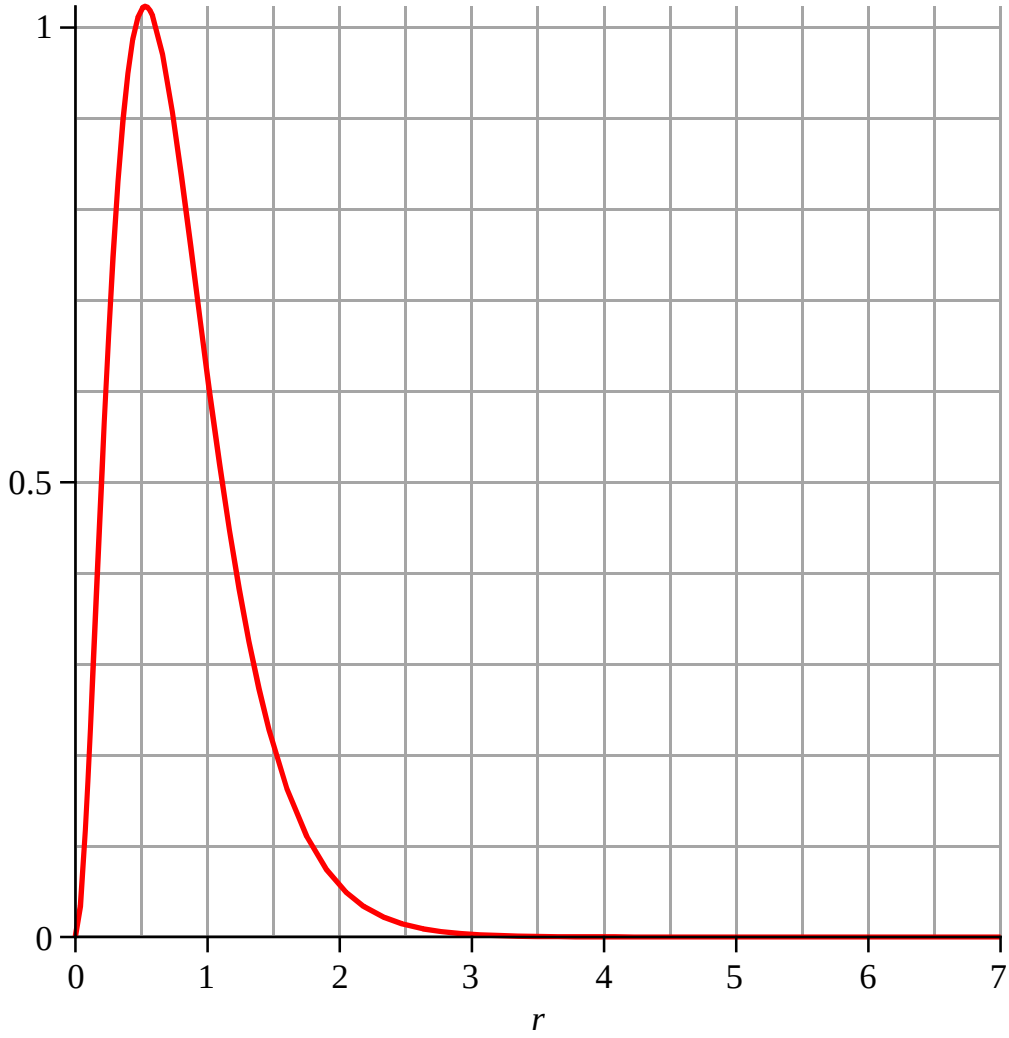
Radial Function and Radial Distribution

```
> graph2 := proc(n, l)
    local g1, g2, h, v, tk, N;
    global a;
    a := 0.529; h := 1; v := 1;
    N := 7·n; tk := 10;
    if n = 4 then tk := 15 end if;
    g1 := plot(R(n, l), r = 0 ..N,
        color = red, legend = [ ' R[n, l](r) '], thickness = 2) :
    g2 := plot(P(n, l), r = 0 ..N,
        color = blue, legend = [' r^2 |R[n, l](r)|^2 ' ], thickness = 2 ) :
    a :='a';
    display([g1, g2], axis[1] = [gridlines = [14·v, linestyle = solid]],
        axis[2] = [gridlines = [12·h, linestyle = solid]], tickmarks = [tk, 3]);
end proc:
```

```
> graph(1, 0); 'R[1, 0]( r)'= R(1, 0);
```

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

```
> graphP(1, 0);
'r^2·(abs(R[1, 0](r)))^2';
 a := 0.529 :
'∫_0^∞ r^2 |R(1, 0)|^2 dr '= ∫_0^∞ r^2 |R(1, 0)|^2 dr;
```



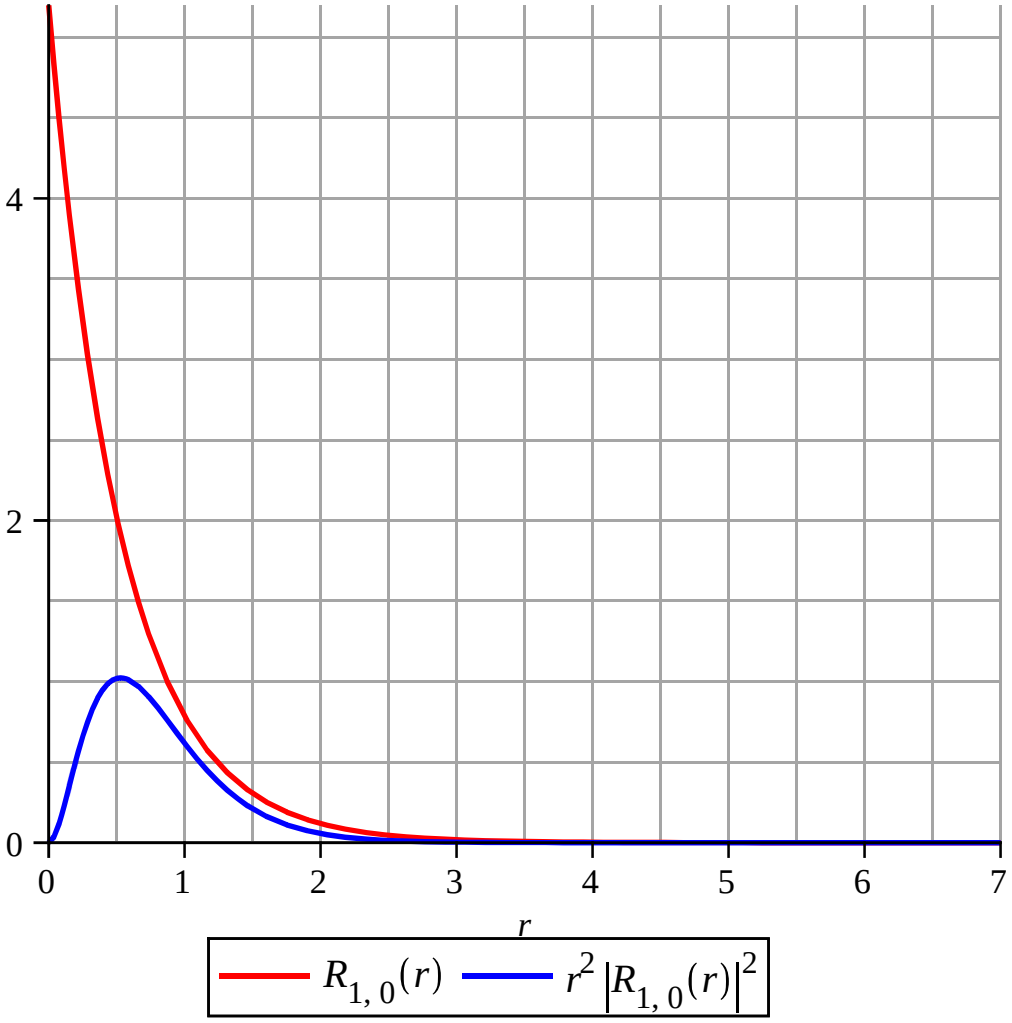
$$r^2 \left|R_{1,\,0}(r)\right|^2$$

$$\int_0^\infty r^2 \left|R(1,\,0)\right|^2 dr = 1.000 \qquad \textbf{(2)}$$

```
> r[max] := max(solve( d/dr (r^2 (R(1, 0))^2) = 0 ));
r[max] :='r[max]': a :='a':
```

$$r_{max} := 0.529 \qquad \textbf{(3)}$$

```
> graph2(1, 0);
```



```
> graph(2, 0);
'R[2, 0]( r)'= (R(2, 0));
```

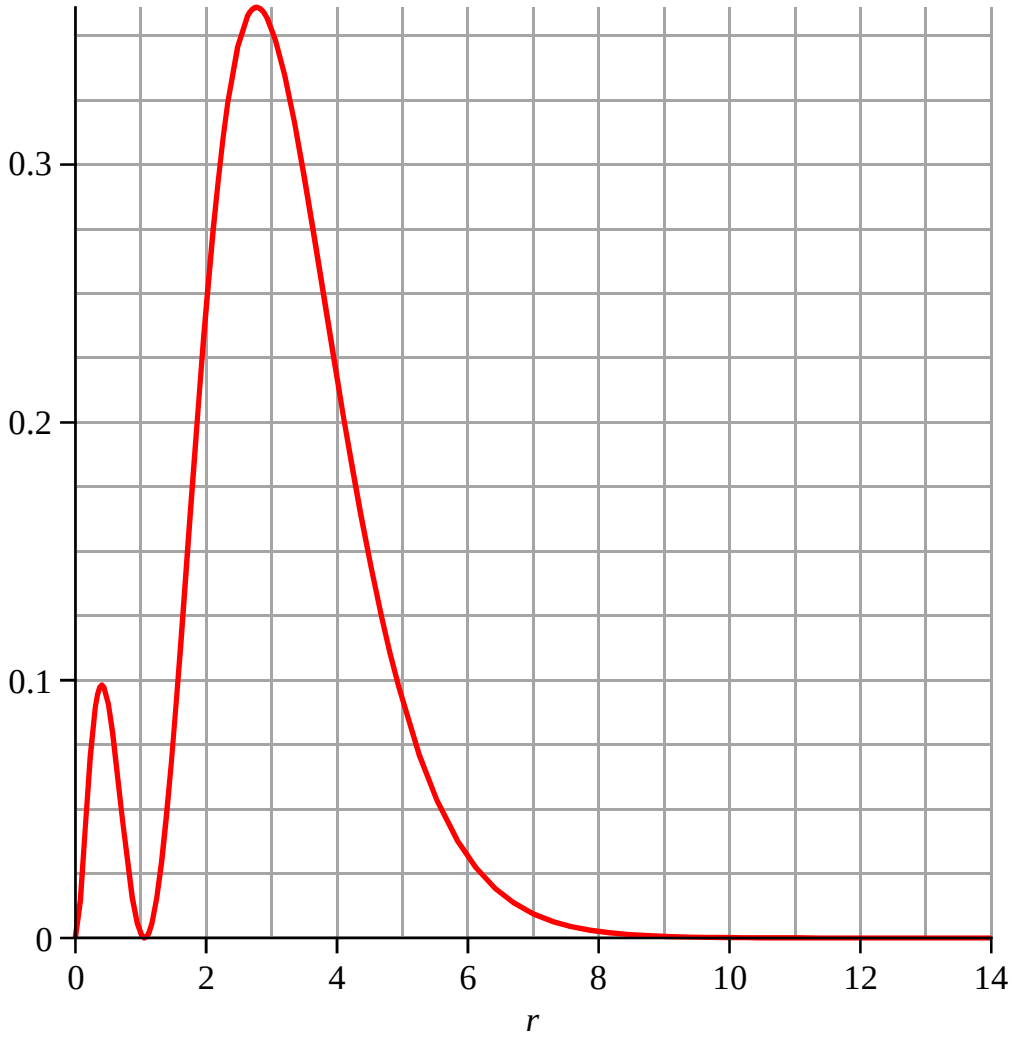
$$R_{2,\,0}(r) = -\frac{1}{4}\,\frac{\sqrt{2}\left(\frac{1}{a}\right)^{3/2} e^{-\frac{1}{2}\frac{r}{a}}\,(-2a + r)}{a} \qquad \textbf{(4)}$$

> *graphP*(2, 0);

'$r^2 \cdot (\mathrm{abs}(R[2,0](r)))^2$';

$a := 0.529$:

$$'\int_0^{\infty} r^2 |R(2,0)|^2 \, dr' = \int_0^{\infty} r^2 |R(2,0)|^2 \, dr;$$



$$r^2 \left|R_{2,0}(r)\right|^2$$

$$\int_0^{\infty} r^2 |R(2,0)|^2 \, dr = 1.000 \qquad \textbf{(5)}$$

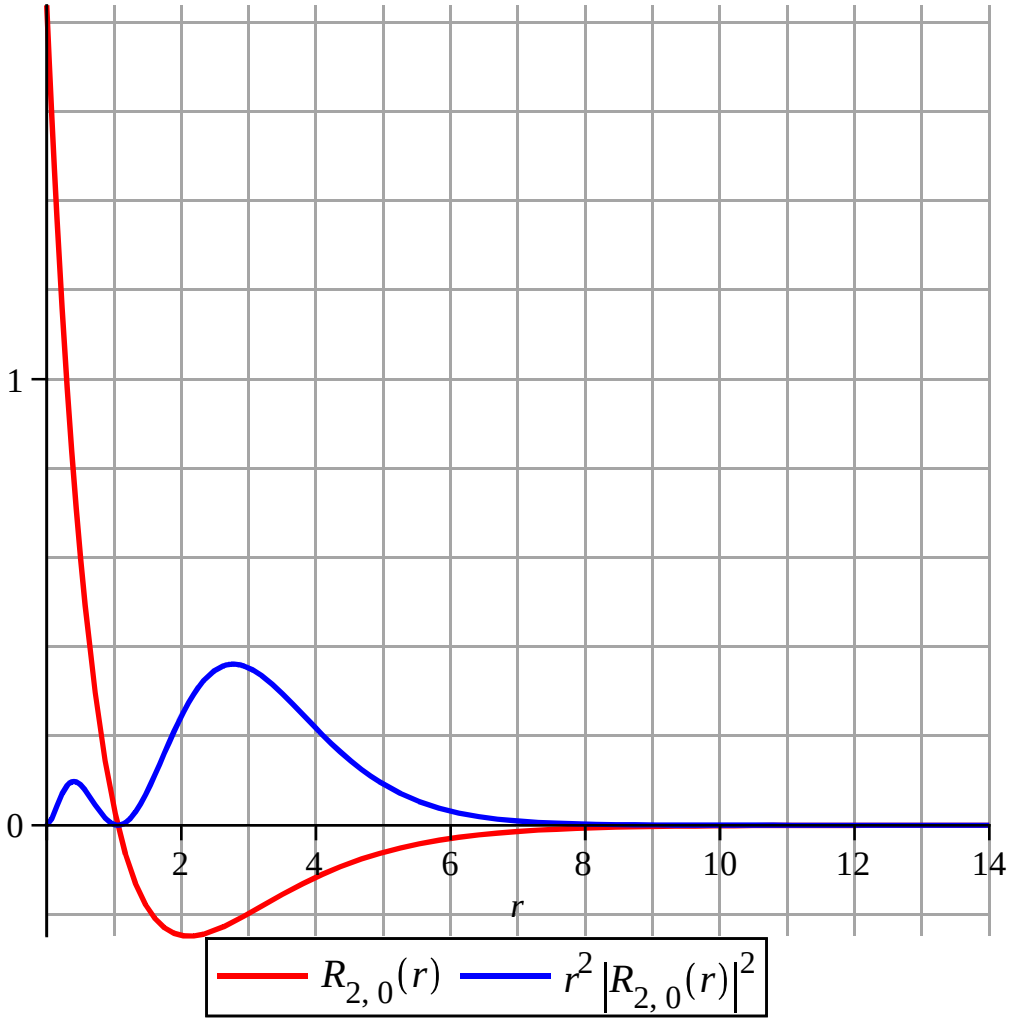
> $r[\max][1] := fsolve\left(\frac{d}{dr}\left(r^2 (R(2,0))^2\right) = 0, r, 0..1\right)$; ; r :='r':

$r[\max][2] := fsolve\left(\frac{d}{dr}\left(r^2 (R(2,0))^2\right) = 0, r, 1..14\right)$; r :='r': a :='a':

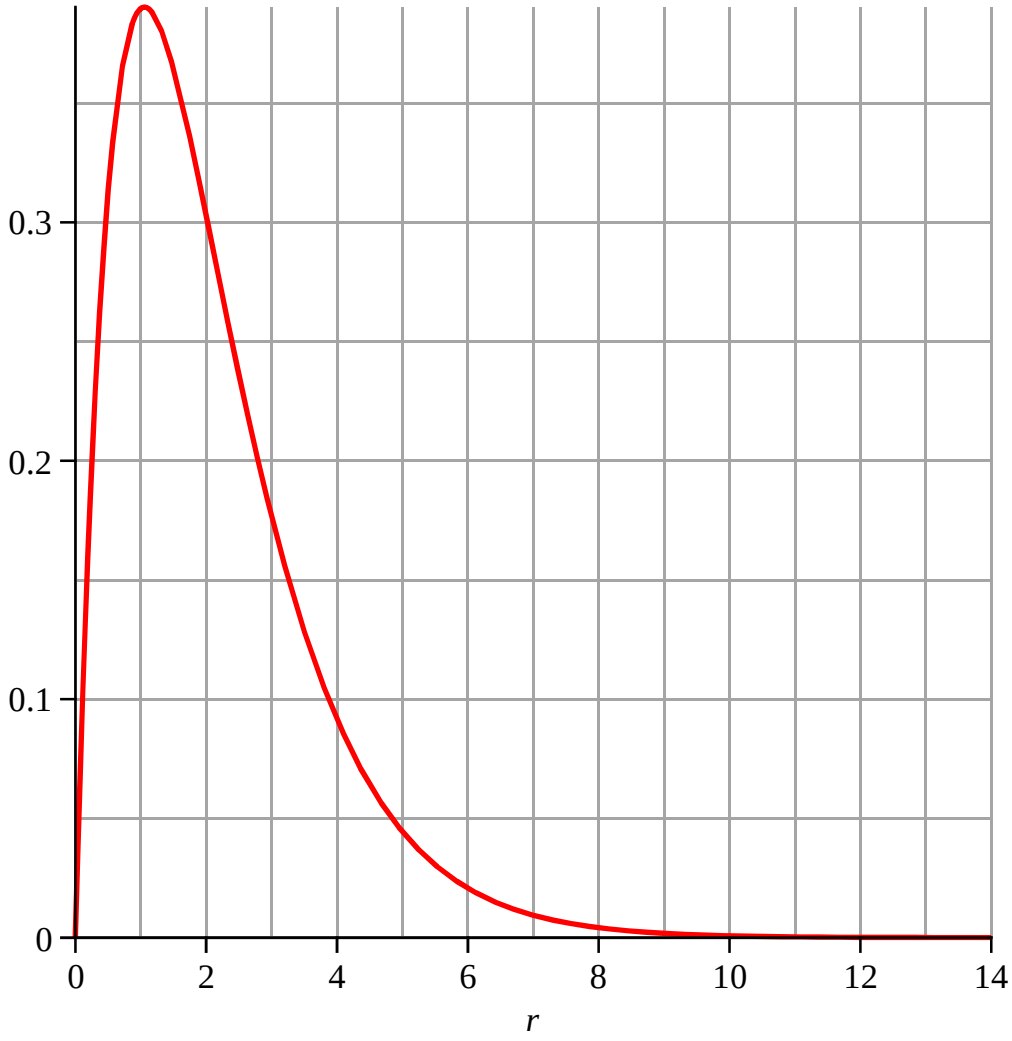
$$r_{\max_1} := 0.404$$

$$r_{\max_2} := 2.770 \qquad \textbf{(6)}$$

```
> graph2(2, 0);
```

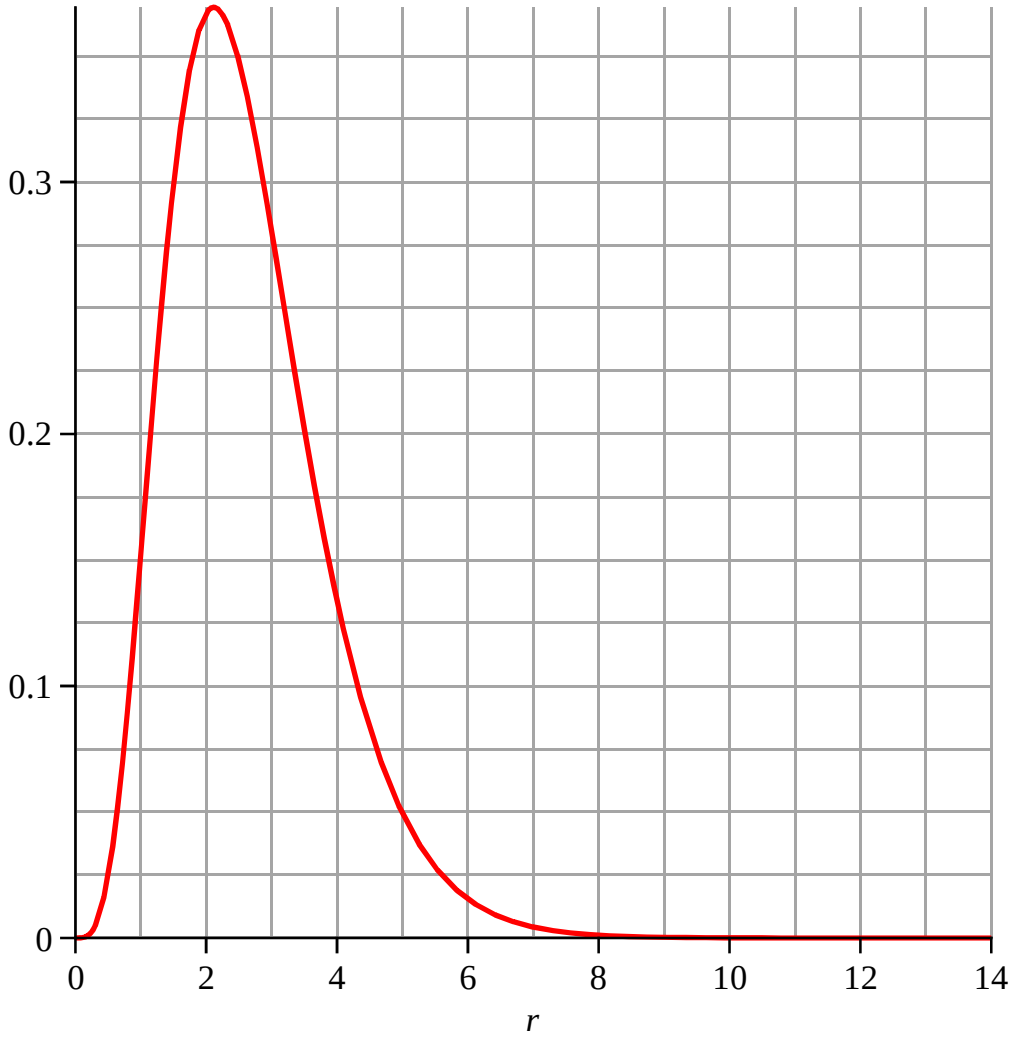


```
> graph(2, 1);
'R[2, 1]( r)'= (R(2, 1));
```



$$R_{2,\,1}(r) = \frac{1}{12}\,\frac{\left(\frac{1}{a}\right)^{3/2}\sqrt{6}\;e^{-\frac{1}{2}\,\frac{r}{a}}\;r}{a} \qquad \textbf{(7)}$$

```
> graphP(2, 1);
'r^2·(abs(R[2, 1](r)))^2';
 a := 0.529 :
'∫_0^∞ r^2 |R(2, 1)|^2 dr '= ∫_0^∞ r^2 |R(2, 1)|^2 dr;
```



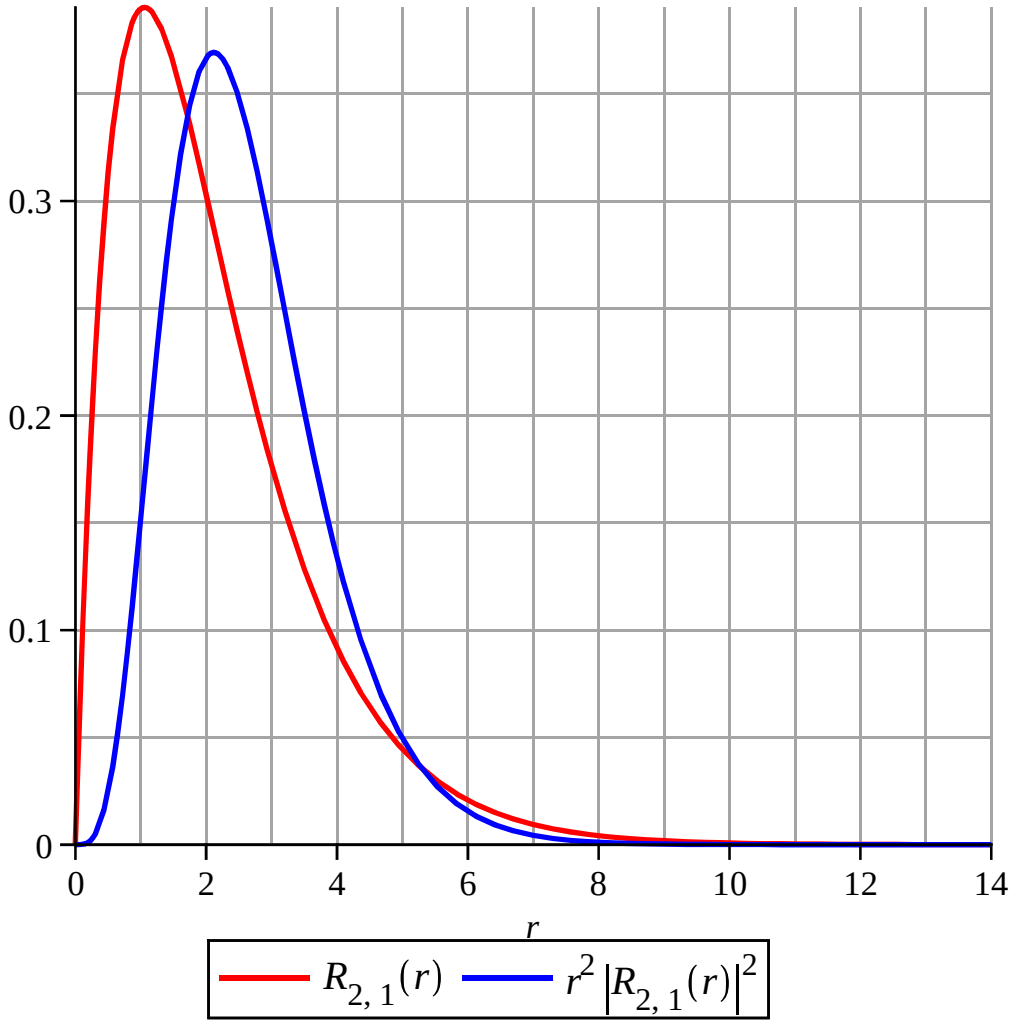
$$r^2 \left|R_{2,\,1}(r)\right|^2$$

$$\int_0^{\infty} r^2 \left|R(2,\,1)\right|^2 dr = 1.000 \qquad \textbf{(8)}$$

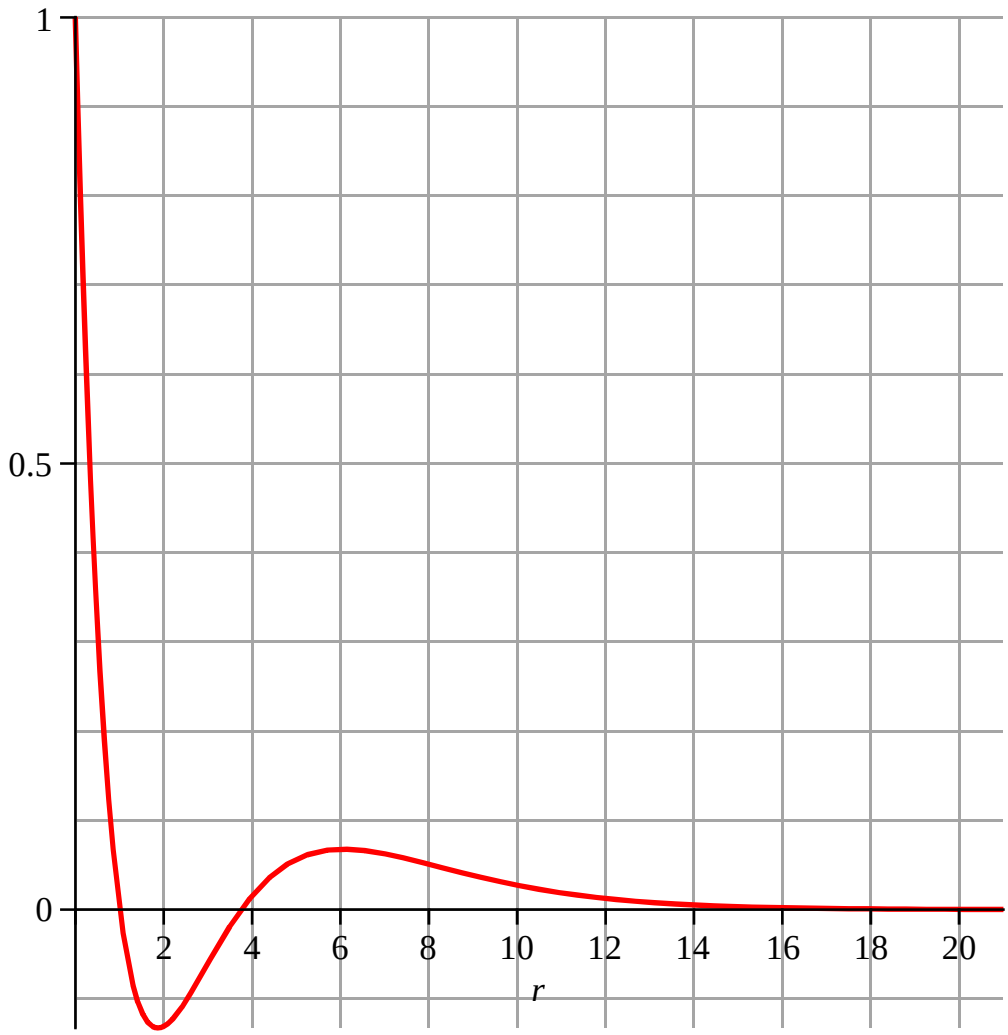
```
> r[max] := max(solve( d/d r (r^2 (R(2, 1))^2) = 0 ));
r[max] :='r[max]': a :='a':
```

$$r_{max} := 2.116 \qquad \textbf{(9)}$$

```
> graph2(2, 1);
```

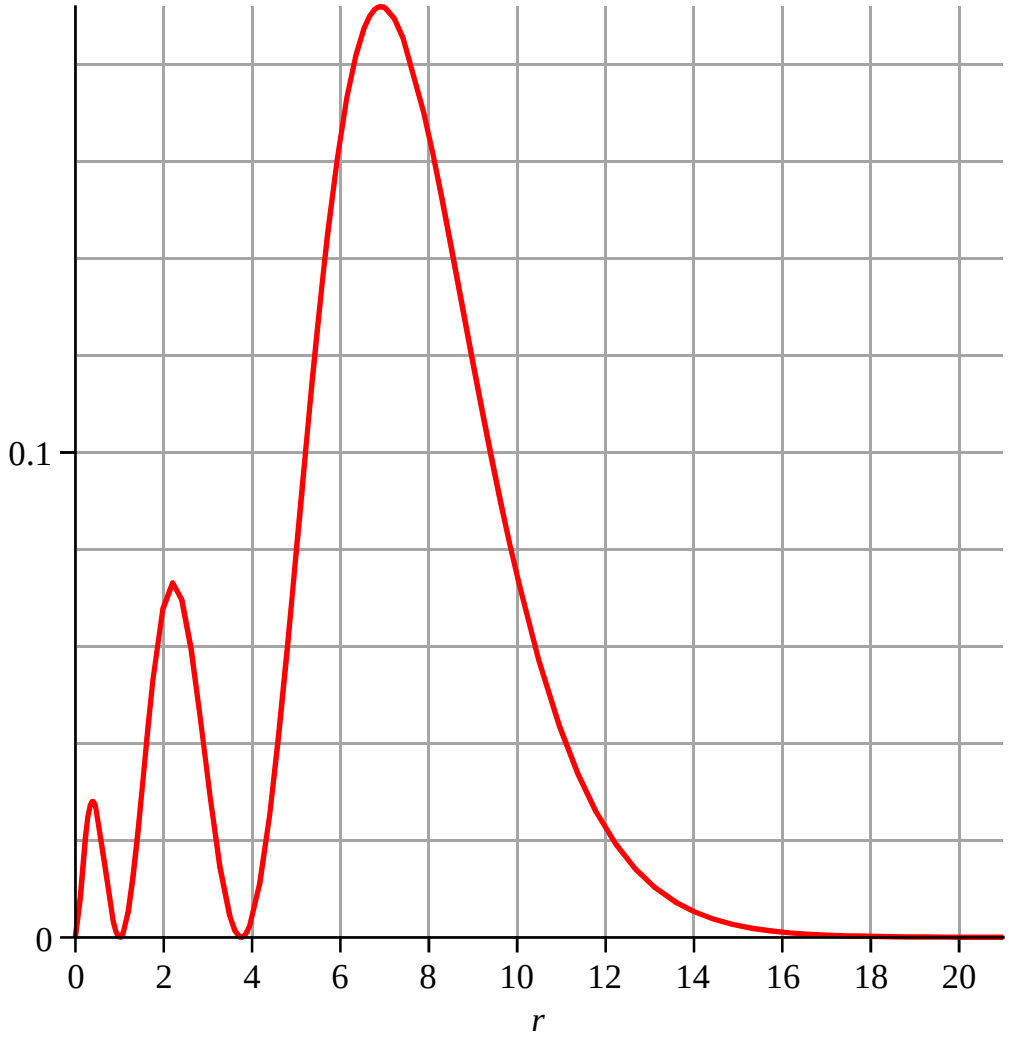


```
> graph(3, 0);
'R[3, 0]( r)'= R(3, 0);
```



$$R_{3,\,0}(r) = \frac{2}{243}\,\frac{\sqrt{3}\left(\frac{1}{a}\right)^{3/2} e^{-\frac{1}{3}\frac{r}{a}}\left(27\,a^2 - 18\,r\,a + 2\,r^2\right)}{a^2} \qquad \textbf{(10)}$$

```
> graphP(3, 0);
'r^2·(abs(R[3, 0](r)))^2';
 a := 0.529 :
'∫_0^∞ r^2 |R(3, 0)|^2 dr '= ∫_0^∞ r^2 |R(3, 0)|^2 dr;
```



$$r^2 \left|R_{3,\,0}(r)\right|^2$$

$$\int_0^\infty r^2 \left|R(3,\,0)\right|^2 dr = 1.000 \qquad \textbf{(11)}$$

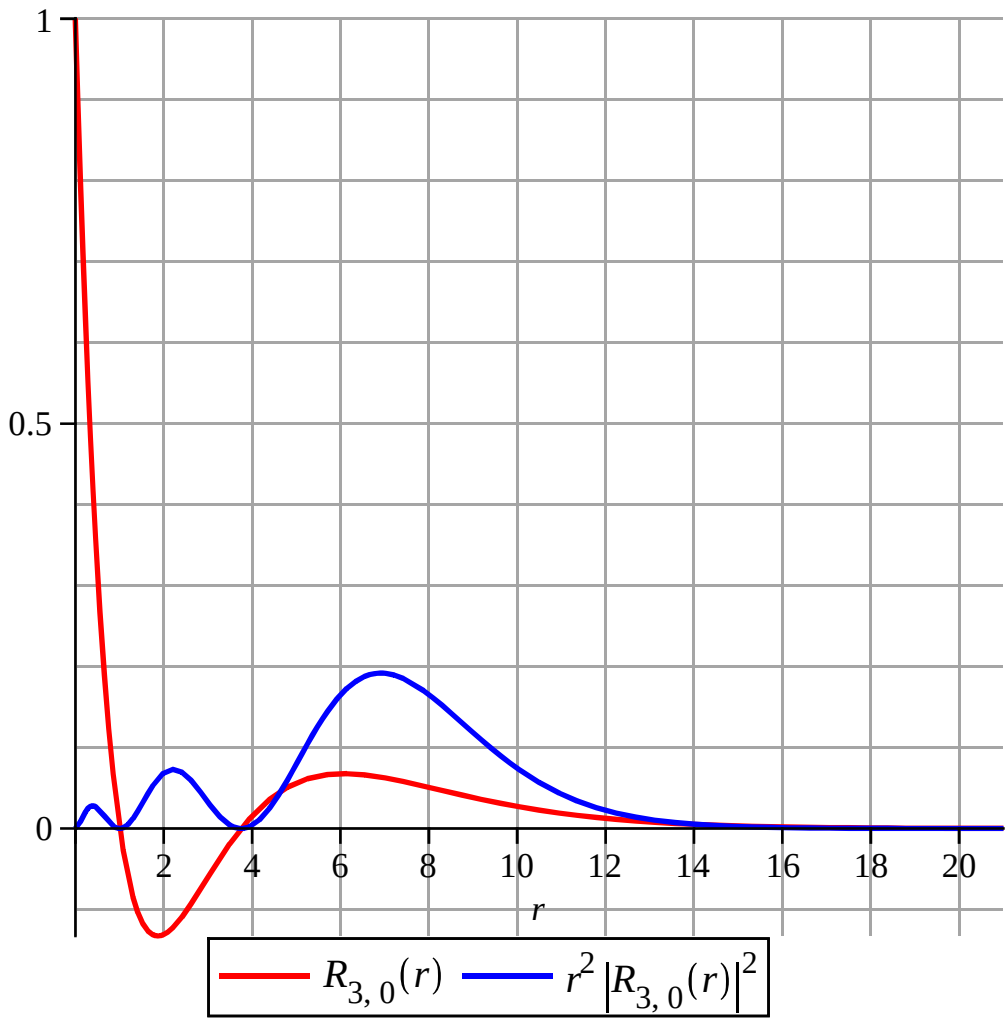
```
> r[max][1] := fsolve( d/d r (r^2 (R(3, 0))^2) = 0, r, 0..1 ); ; r :='r':
 r[max][2] := fsolve( d/d r (r^2 (R(3, 0))^2) = 0, r, 1..4 ); ; r :='r':
r[max][3] := fsolve( d/d r (r^2 (R(3, 0))^2) = 0, r, 4..20 ); r :='r': a :='a':
```

$$r_{max_1} := 0.391$$

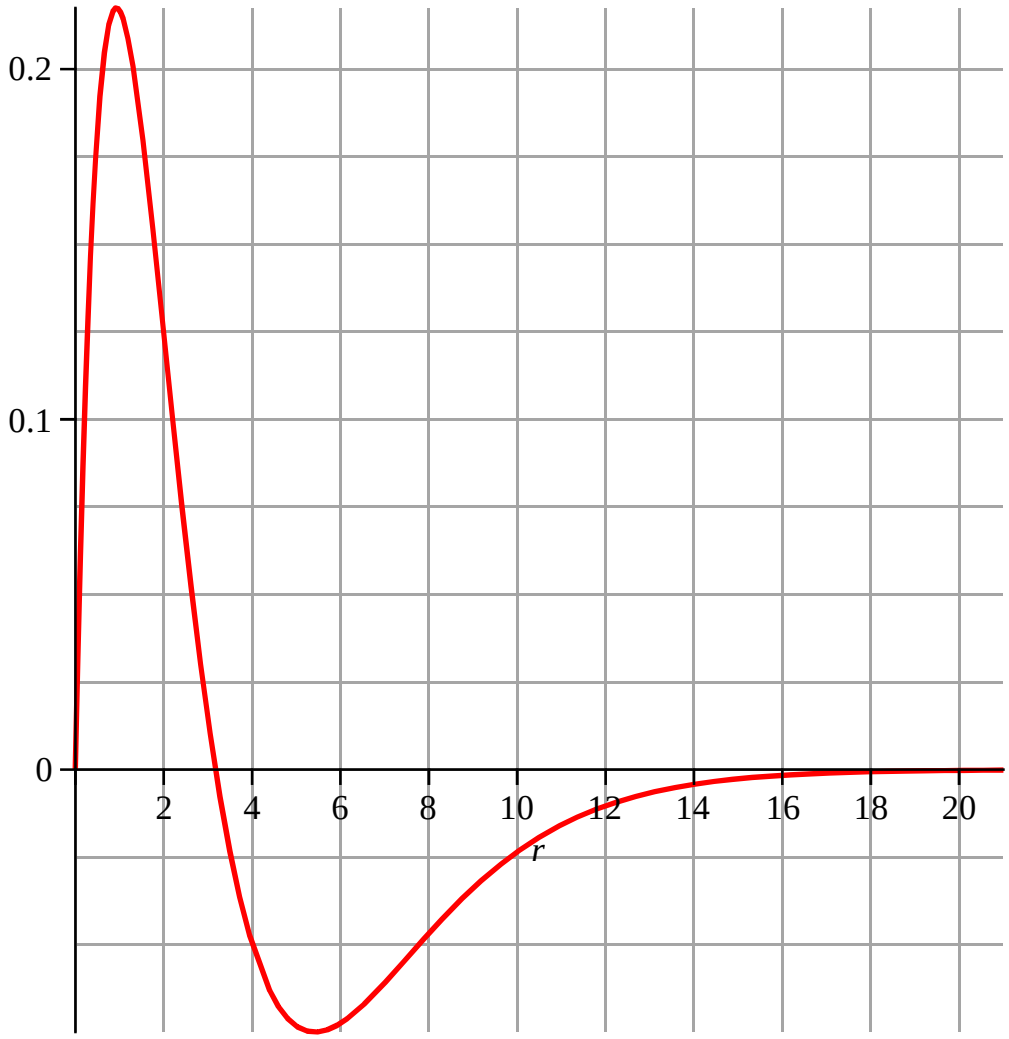
$$r_{max_2} := 2.214$$

$$r_{max_3} := 6.916 \qquad \textbf{(12)}$$

```
> graph2(3, 0);
```



```
> graph(3, 1);
'R[3, 1]( r)'= R(3, 1);
```



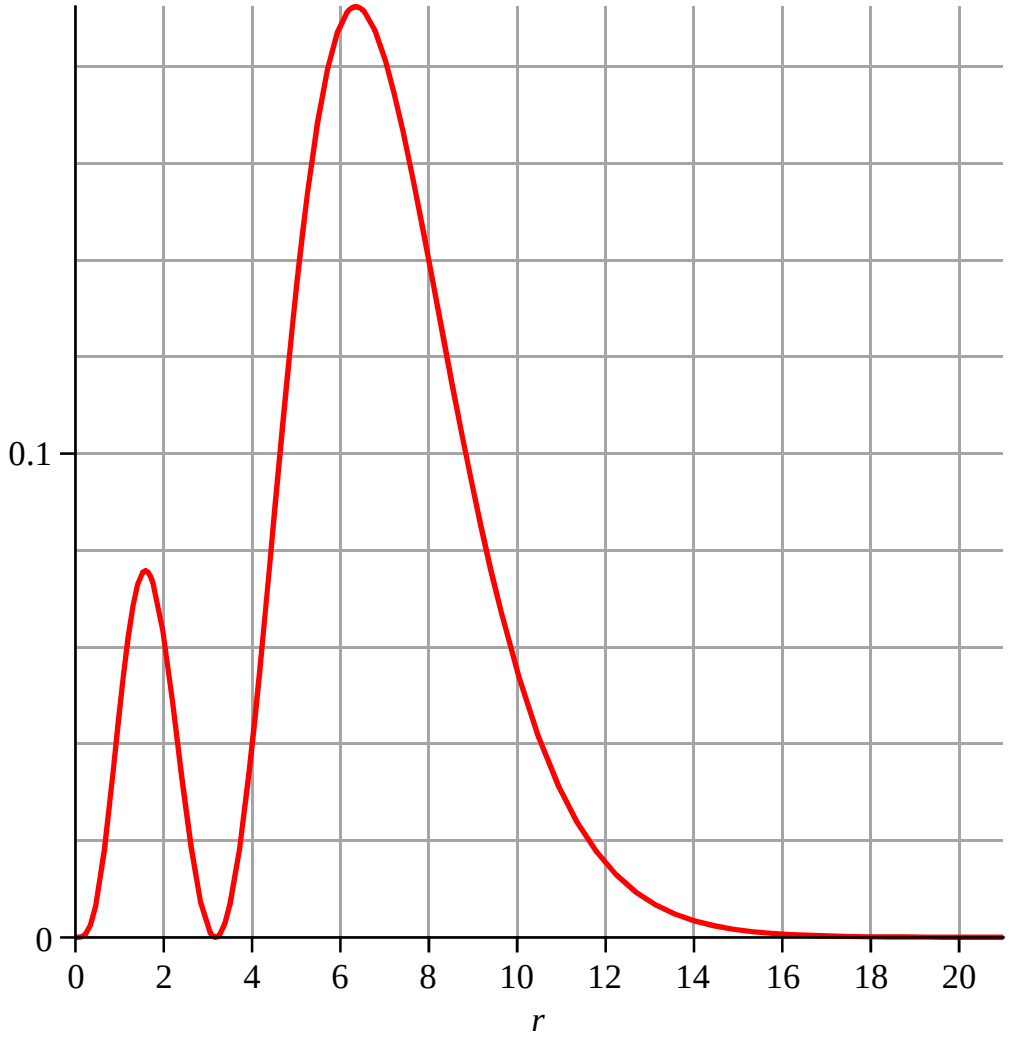
$$R_{3,\,1}(r) = \frac{2}{243}\,\frac{\sqrt{2}\,\sqrt{3}\,\left(\frac{1}{a}\right)^{3/2}\,e^{-\frac{1}{3}\,\frac{r}{a}}\,r\,(6\,a - r)}{a^2} \qquad \textbf{(13)}$$

> *graphP*(3, 1);

'$r^2 \cdot (\mathrm{abs}(R[3, 1](r)))^2$';

$a := 0.529$:

'$\int_0^\infty r^2 |R(3, 1)|^2 \, dr$' = $\int_0^\infty r^2 |R(3, 1)|^2 \, dr$;



$r^2 |R_{3, 1}(r)|^2$

$$\int_0^\infty r^2 |R(3, 1)|^2 \, dr = 1.000 \quad \textbf{(14)}$$

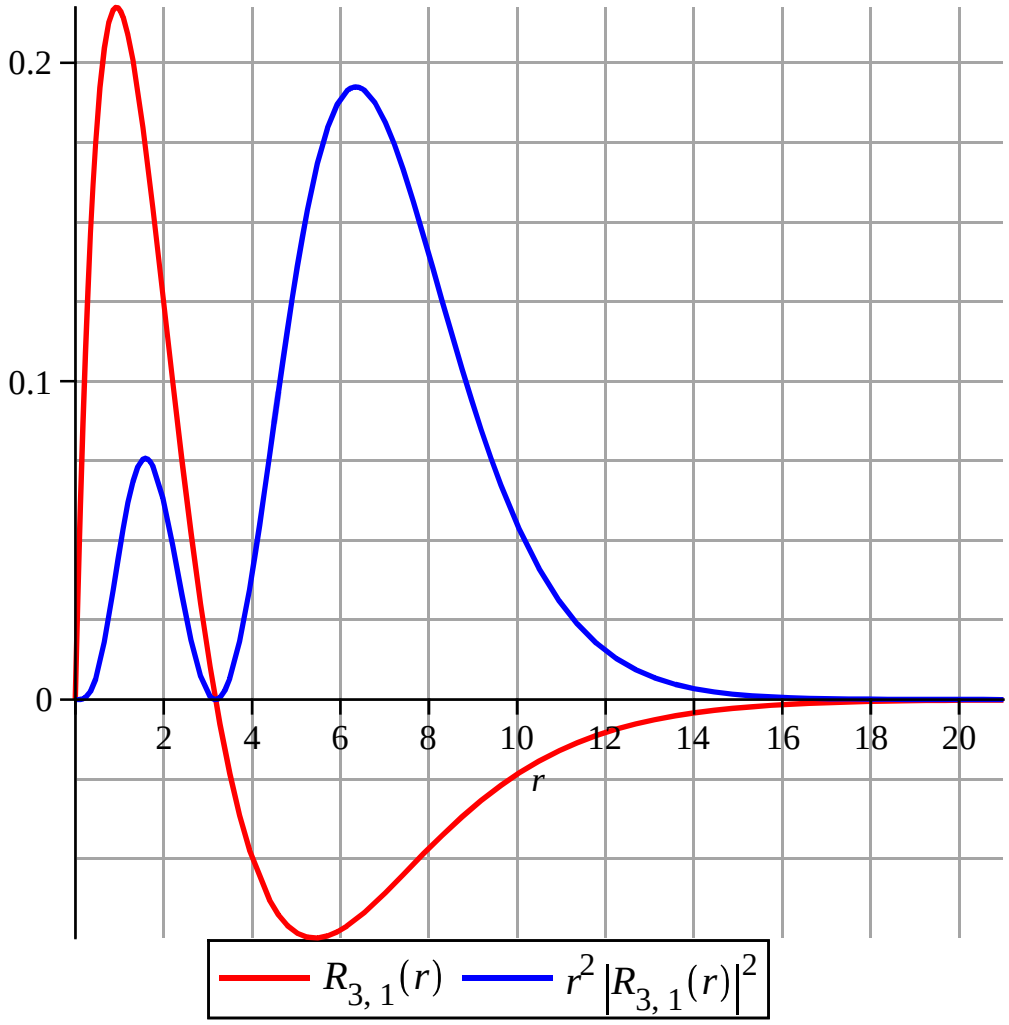
> r[max][1] := *fsolve*$\left(\frac{d}{d\,r}\left(r^2 (R(3, 1))^2\right) = 0, r, 0..3\right)$; ; r := 'r':

r[max][2] := *fsolve*$\left(\frac{d}{d\,r}\left(r^2 (R(3, 1))^2\right) = 0, r, 3..20\right)$; r := 'r': a := 'a':

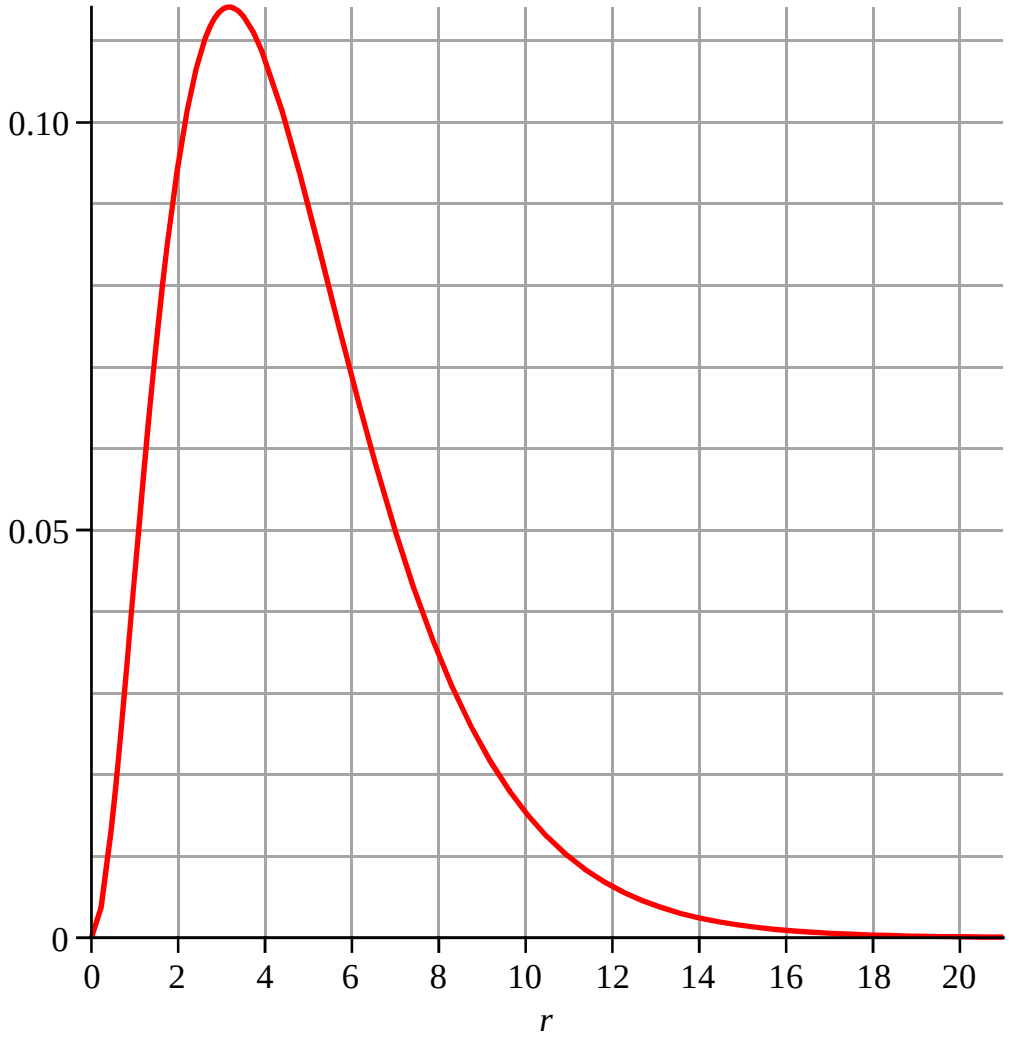
$r_{max_1} := 1.587$

$r_{max_2} := 6.348$ **(15)**

```
> graph2(3, 1);
```

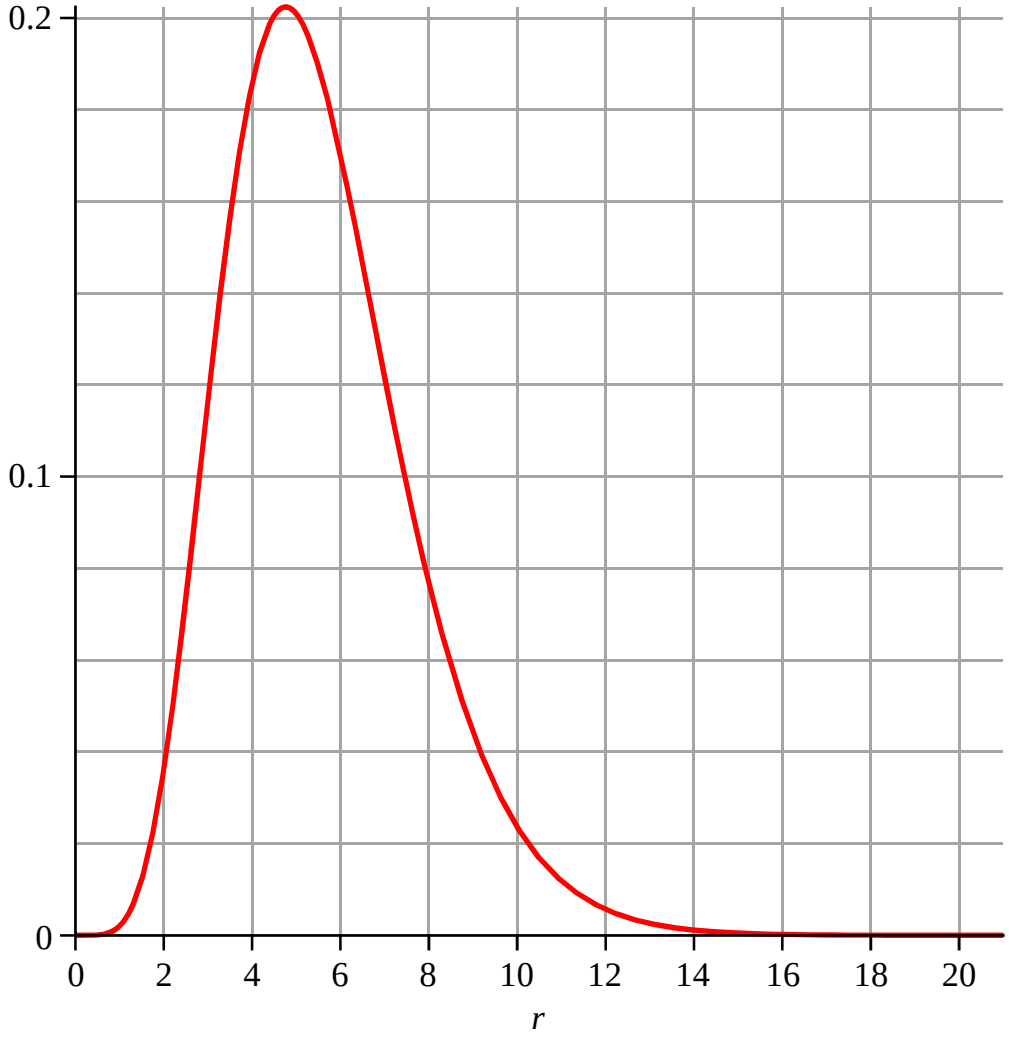


```
> graph(3, 2);
'R[3, 2]( r)'= R(3, 2);
```



$$R_{3,\,2}(r) = \frac{2}{1215}\,\frac{\sqrt{2}\,\sqrt{3}\left(\frac{1}{a}\right)^{3/2}\sqrt{5}\;e^{-\frac{1}{3}\,\frac{r}{a}}\;r^2}{a^2} \qquad \textbf{(16)}$$

```
> graphP(3, 2);
'r^2·(abs(R[3, 2](r)))^2';
 a := 0.529 :
'∫_0^∞ r^2 |R(3, 2)|^2 dr '= ∫_0^∞ r^2 |R(3, 2)|^2 dr;
```



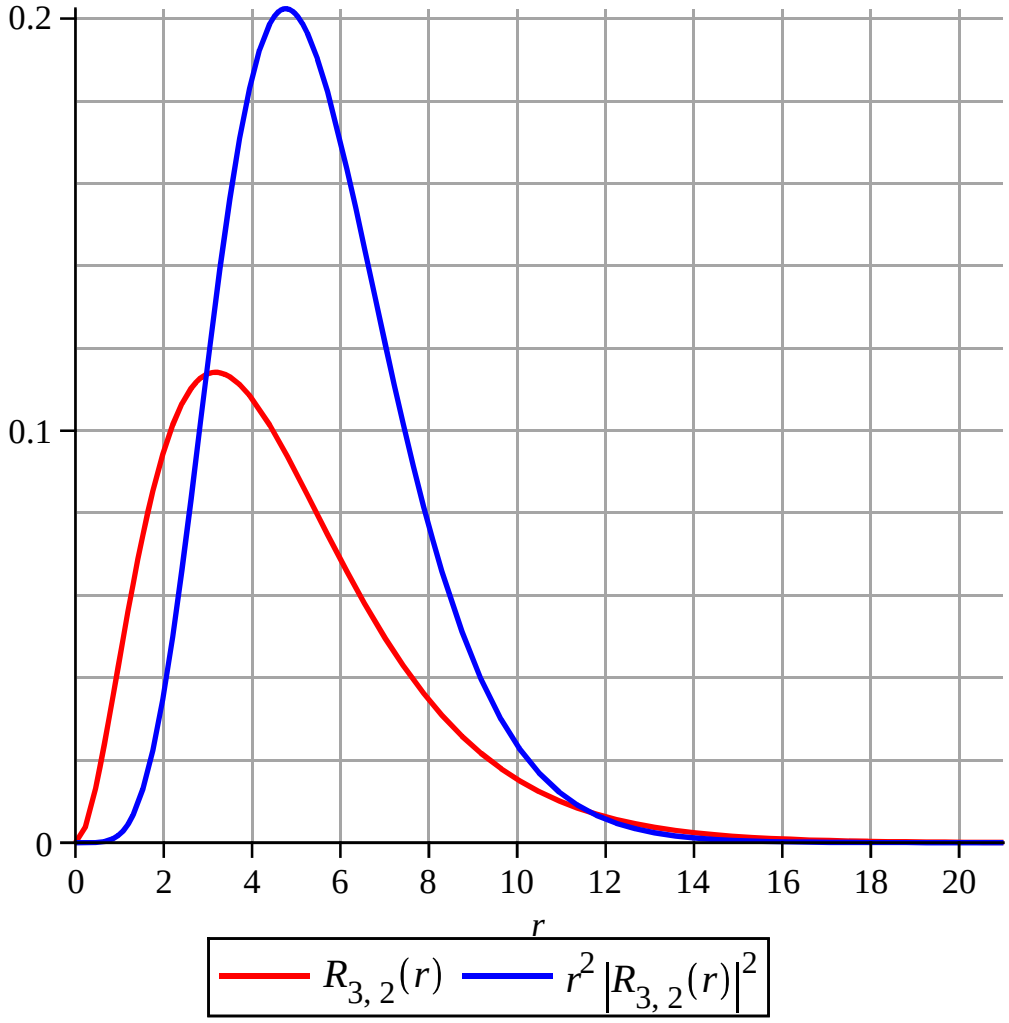
$$r^2 \left|R_{3,\,2}(r)\right|^2$$

$$\int_0^\infty r^2 \left|R(3,\,2)\right|^2 dr = 1.000 \qquad \textbf{(17)}$$

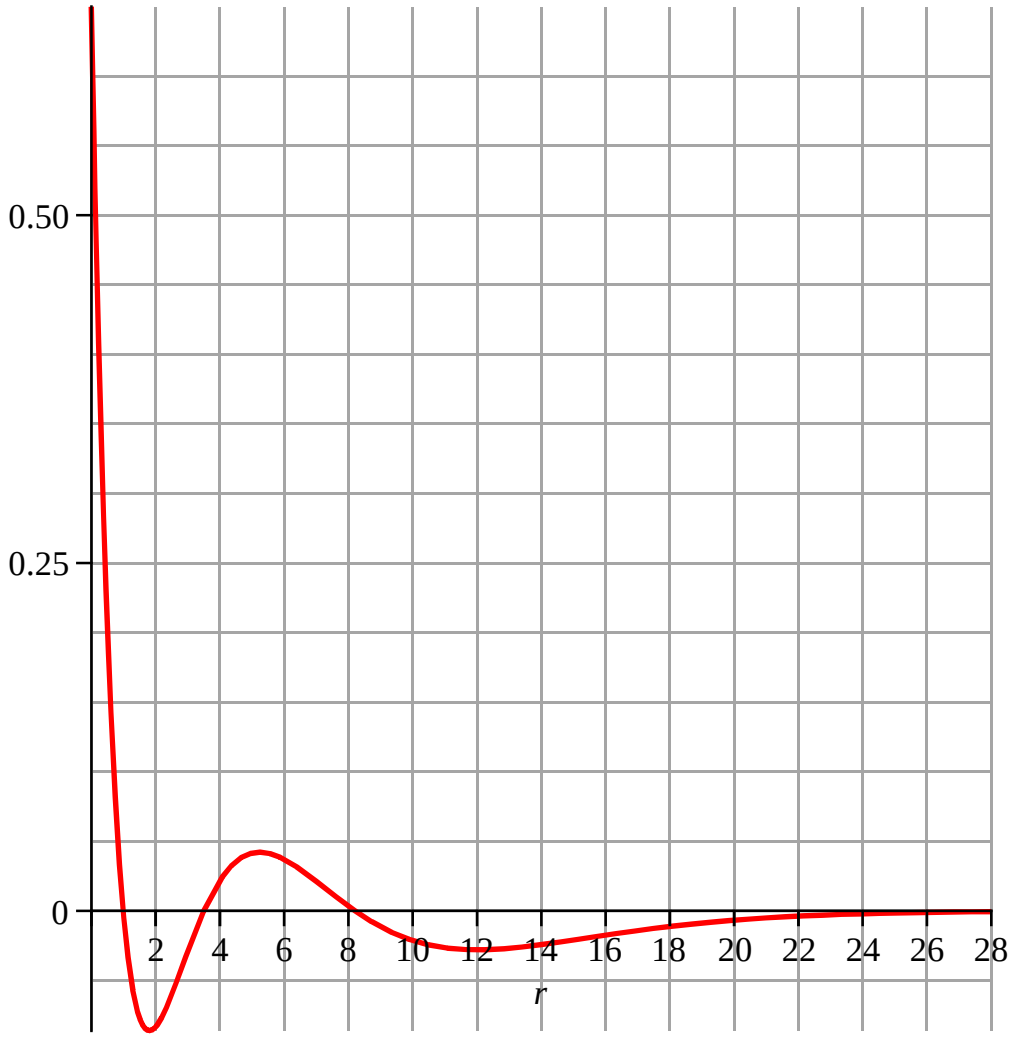
```
> r[max] := max(solve( d/dr (r^2 (R(3, 2))^2) = 0 ));
r[max] :='r[max]': a :='a':
```

$$r_{max} := 4.761 \qquad \textbf{(18)}$$

```
> graph2(3, 2);
```



```
> graph(4, 0);
'R[4, 0]( r)'= R(4, 0);
```



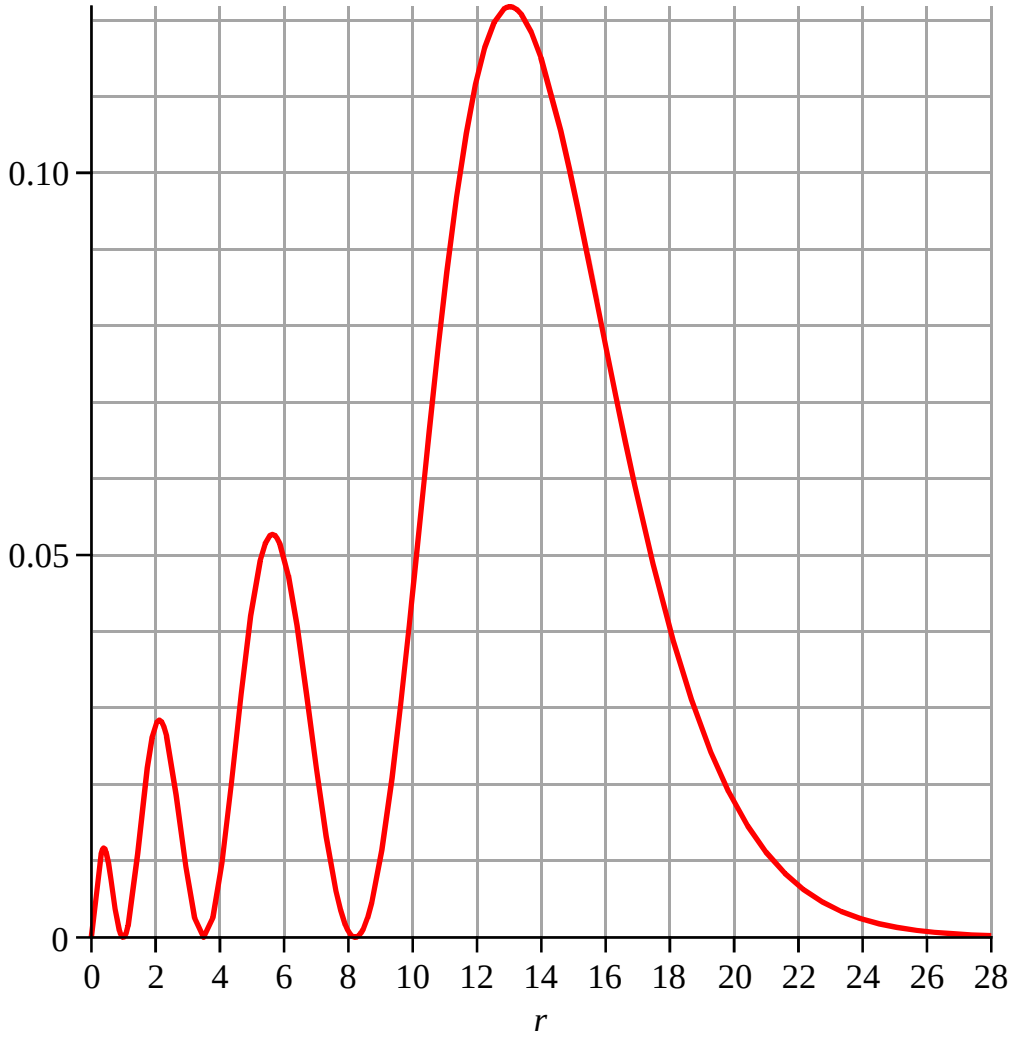
$$R_{4,\,0}(r) = -\frac{1}{1536}\,\frac{\sqrt{4}\left(\frac{1}{a}\right)^{3/2} e^{-\frac{1}{4}\frac{r}{a}}\left(-192\,a^3+144\,r\,a^2-24\,r^2\,a+r^3\right)}{a^3} \qquad \textbf{(19)}$$

> *graphP*(4, 0);

'$r^2 \cdot (\mathrm{abs}(R[4, 0](r)))^2$';

$a := 0.529$:

'$\int_0^\infty r^2 |R(4, 0)|^2 \, dr$'$= \int_0^\infty r^2 |R(4, 0)|^2 \, dr$;



$r^2 |R_{4,0}(r)|^2$

$\int_0^\infty r^2 |R(4, 0)|^2 \, dr = 1.000$ **(20)**

> x := *fsolve*$\left(\frac{d}{dr}\left(r^2 (R(4, 0))^2\right) = 0, r, 0..1\right)$: r :='r':

y := *fsolve*$\left(\frac{d}{dr}\left(r^2 (R(4, 0))^2\right) = 0, r, 1..3\right)$: r :='r':

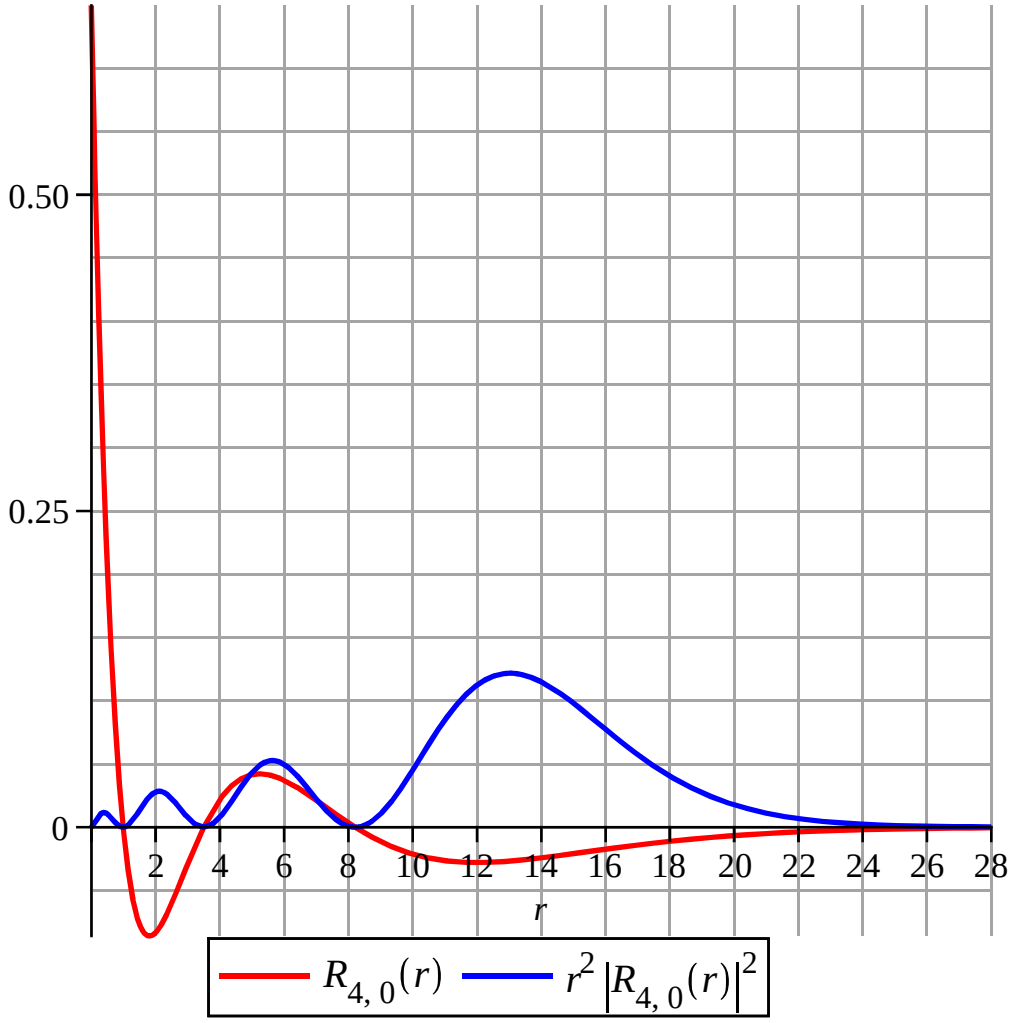
z := *fsolve*$\left(\frac{d}{dr}\left(r^2 (R(4, 0))^2\right) = 0, r, 4..8\right)$: r :='r':

w := *fsolve*$\left(\frac{d}{dr}\left(r^2 (R(4, 0))^2\right) = 0, r, 8..28\right)$: r :='r': a :='a':

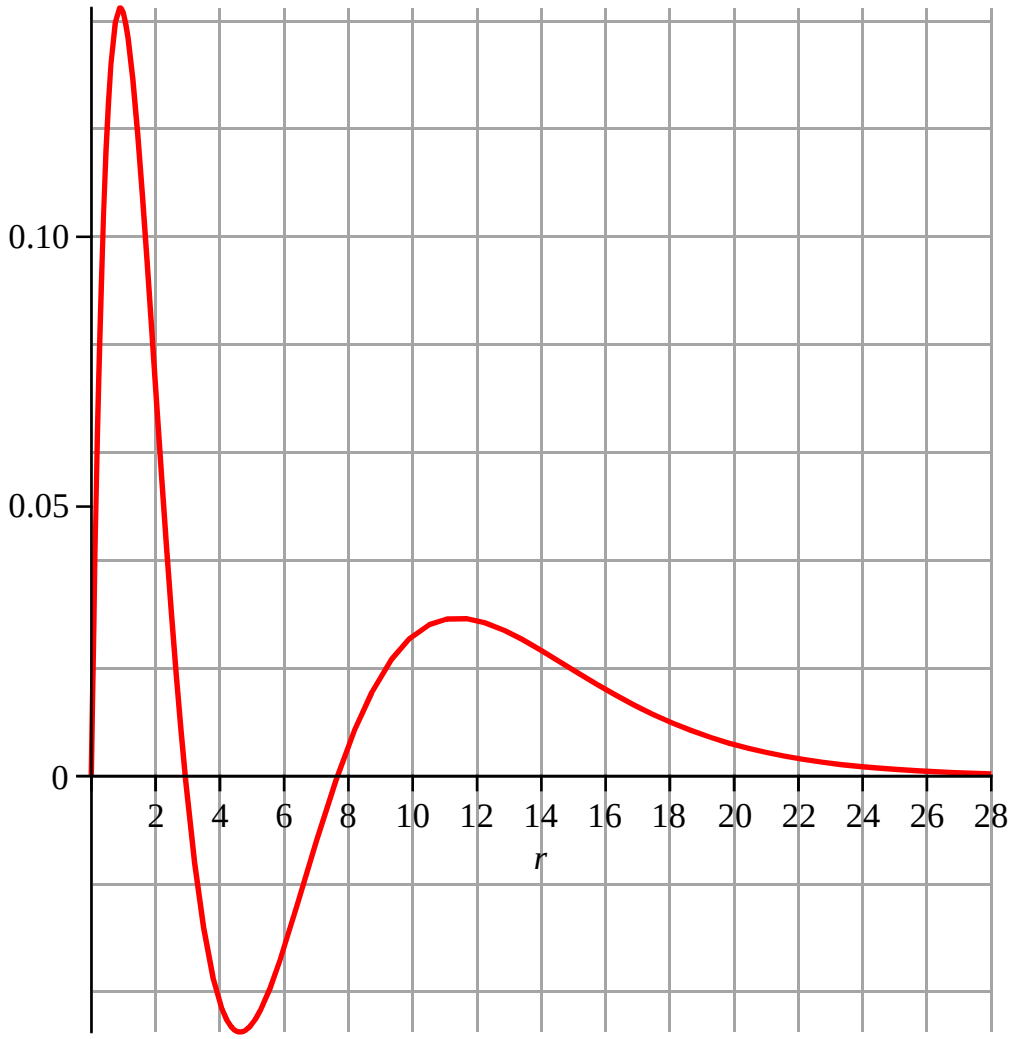
$r[\max] := [x, y, z, w]$;

$r_{\max} := [0.387, 2.116, 5.634, 13.023]$ **(21)**

```
> graph2(4, 0);
```



```
> graph(4, 1);
'R[4, 1]( r)'= combine(R(4, 1));
```



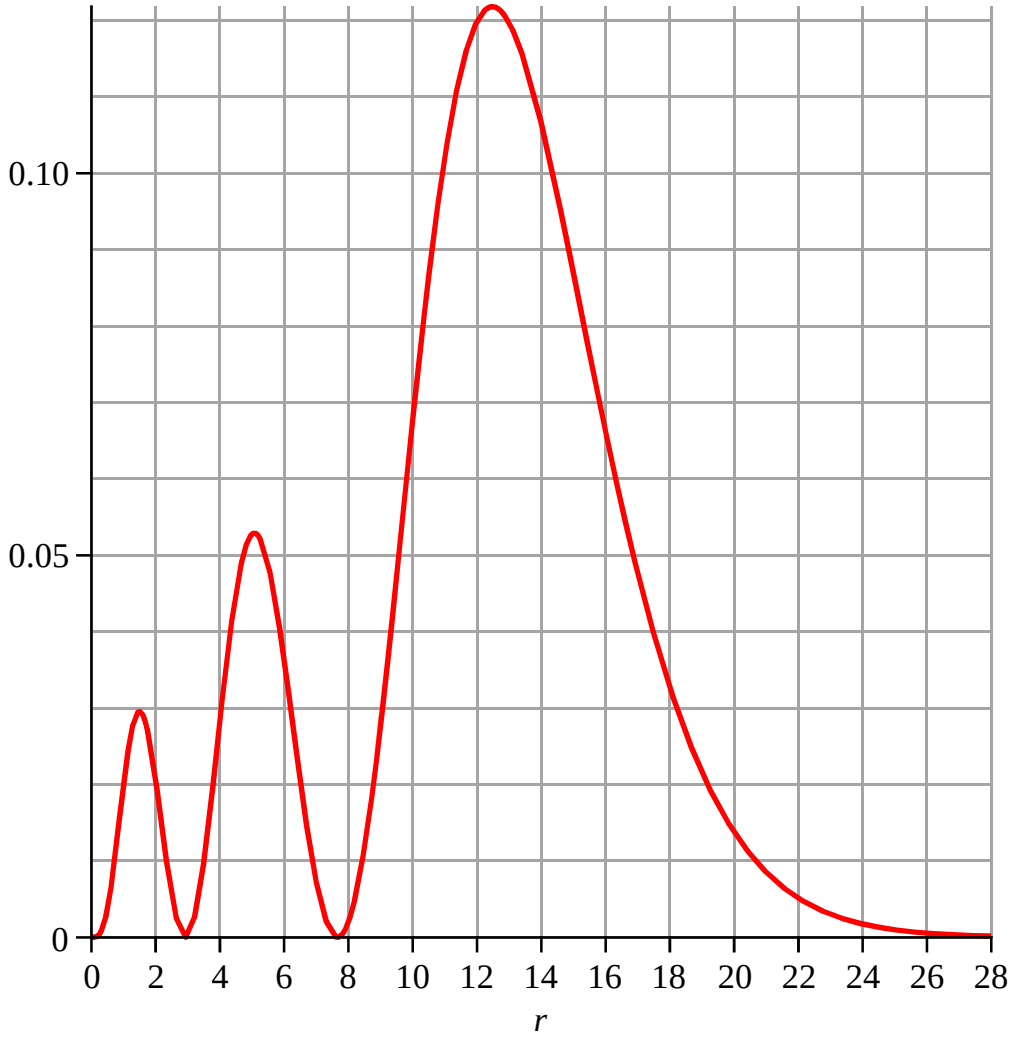
$$R_{4,\,1}(r) = \frac{1}{3840}\,\frac{r\left(80\,a^2 - 20\,r\,a + r^2\right)\sqrt{15}\,\sqrt{\frac{1}{a}}\;e^{-\frac{1}{4}\,\frac{r}{a}}}{a^4} \qquad \textbf{(22)}$$

> *graphP*(4, 1);

'$r^2 \cdot (\mathrm{abs}(R[4,1](r)))^2$';

$a := 0.529$:

$'\int_0^{\infty} r^2 |R(4,1)|^2 \, dr' = \int_0^{\infty} r^2 |R(4,1)|^2 \, dr$;



$$r^2 \left|R_{4,1}(r)\right|^2$$

$$\int_0^{\infty} r^2 |R(4,1)|^2 \, dr = 1.000 \qquad \textbf{(23)}$$

> r[max][1] := *fsolve*$\left(\frac{d}{d\,r}\left(r^2 (R(4,1))^2\right) = 0, r, 0..3\right)$; ; r := 'r':

r[max][2] := *fsolve*$\left(\frac{d}{d\,r}\left(r^2 (R(4,1))^2\right) = 0, r, 3..8\right)$; ; r := 'r':

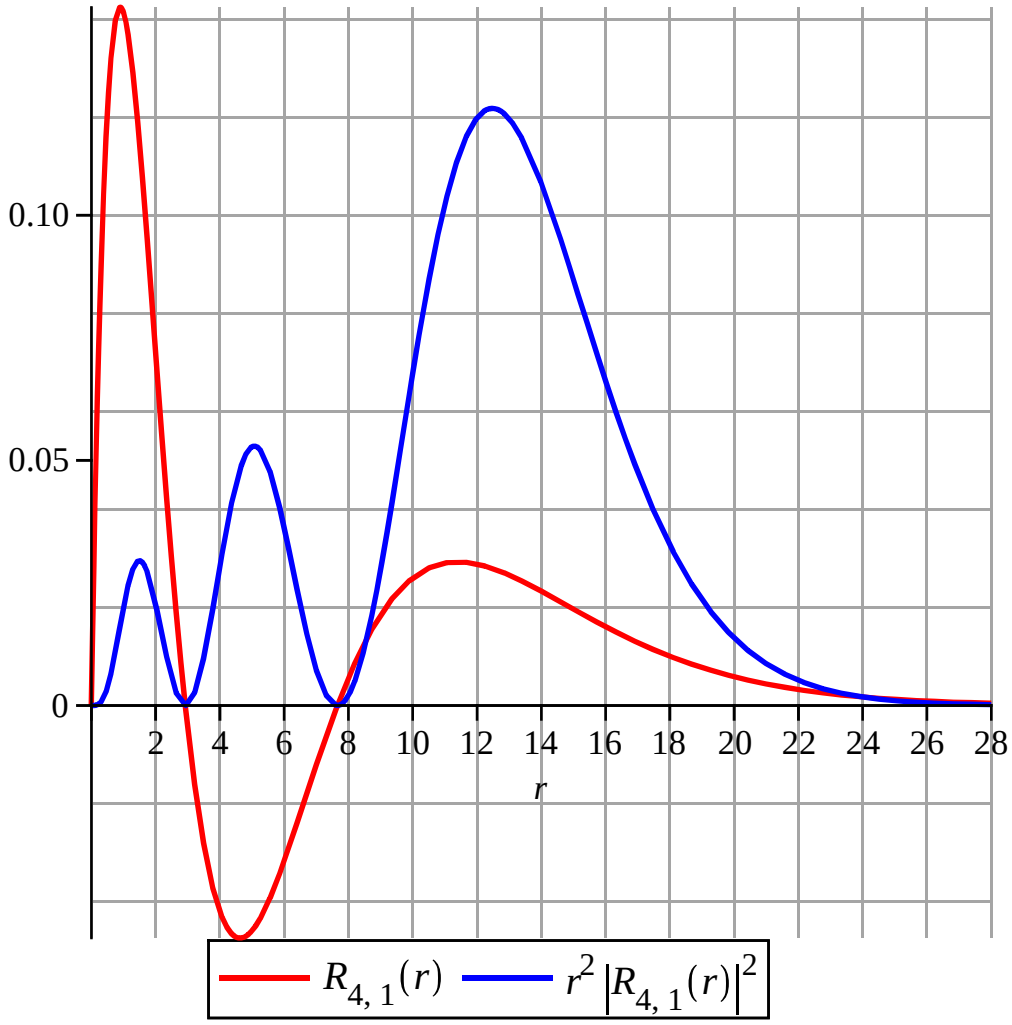
r[max][3] := *fsolve*$\left(\frac{d}{d\,r}\left(r^2 (R(4,1))^2\right) = 0, r, 8..28\right)$; r := 'r': a := 'a':

$$r_{max_1} := 1.497$$

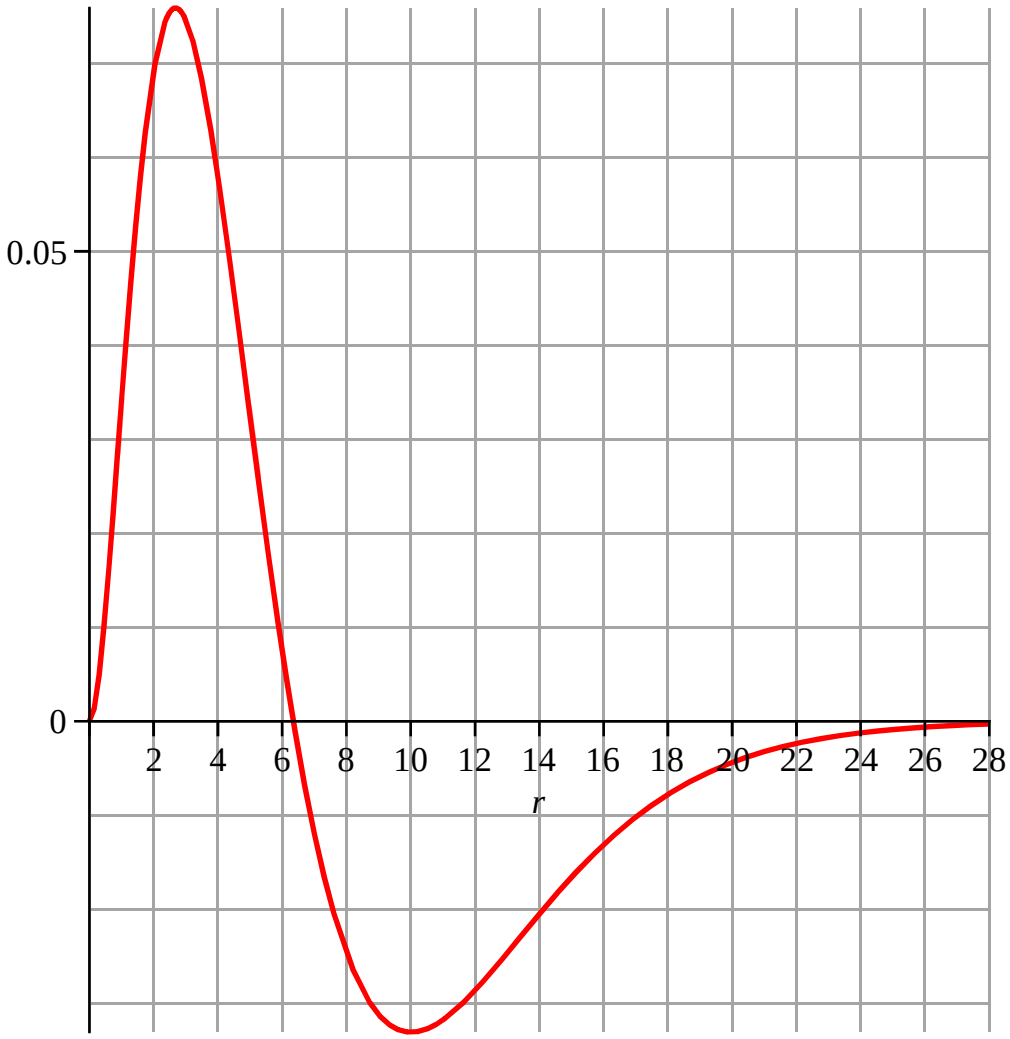
$$r_{max_2} := 5.073$$

$$r_{max_3} := 12.474 \qquad \textbf{(24)}$$

```
> graph2(4, 1);
```



```
> graph(4, 2);
'R[4, 2]( r)'= combine(R(4, 2));
```



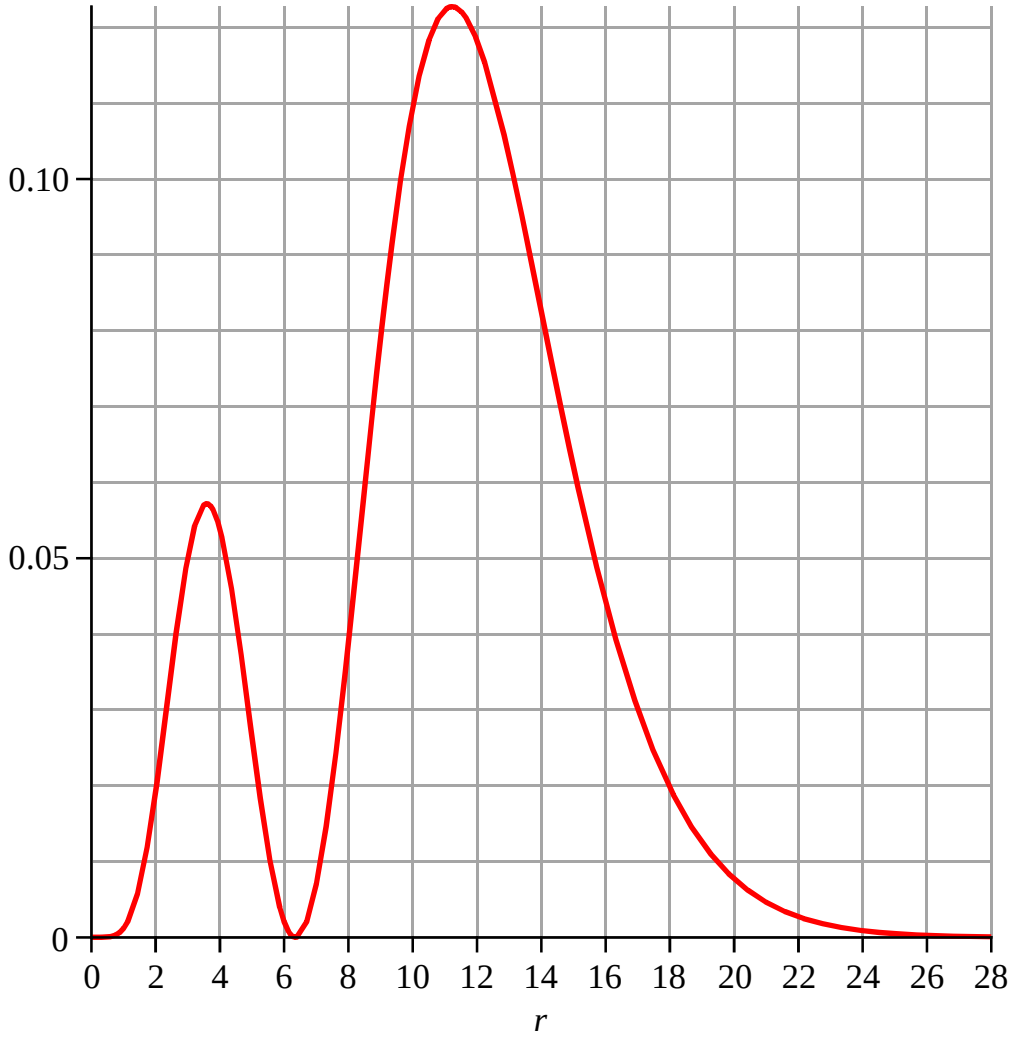
$$R_{4,2}(r) = \frac{1}{3840}\,\frac{r^2\,(12\,a - r)\,\sqrt{5}\,\sqrt{\frac{1}{a}}\,e^{-\frac{1}{4}\,\frac{r}{a}}}{a^4} \qquad \textbf{(25)}$$

> *graphP*(4, 2);

'$r^2 \cdot (\mathrm{abs}(R[4,2](r)))^2$';

$a := 0.529$:

'$\int_0^\infty r^2 |R(4,2)|^2 \, dr$' = $\int_0^\infty r^2 |R(4,2)|^2 \, dr$;



$r^2 |R_{4,2}(r)|^2$

$$\int_0^\infty r^2 |R(4,2)|^2 \, dr = 1.000 \quad \textbf{(26)}$$

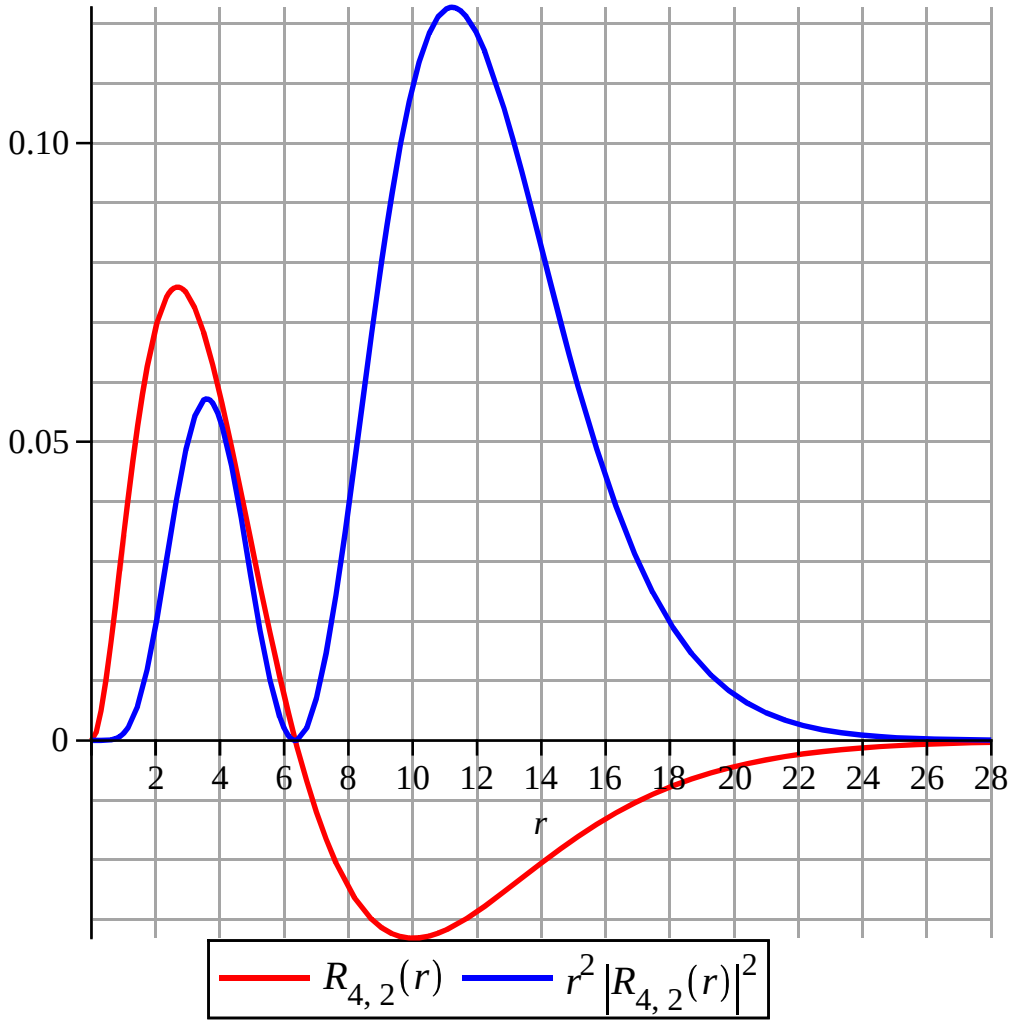
> r[max][1] := *fsolve*$\left(\frac{d}{dr}\left(r^2 (R(4,2))^2\right) = 0, r, 0..6\right)$; ; r :='r':

r[max][2] := *fsolve*$\left(\frac{d}{dr}\left(r^2 (R(4,2))^2\right) = 0, r, 6..28\right)$; r :='r': a :='a':

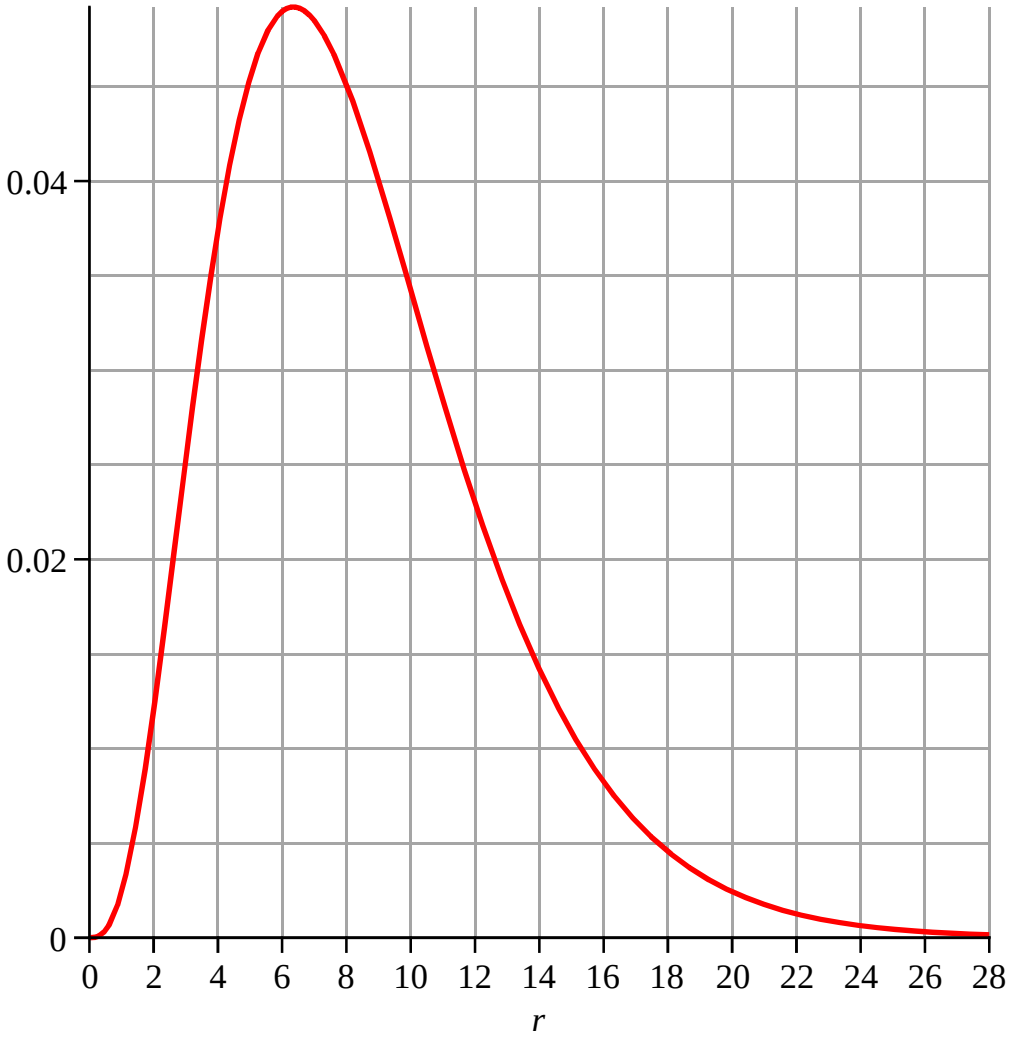
$r_{max_1} := 3.591$

$r_{max_2} := 11.221$ **(27)**

```
> graph2(4, 2);
```



```
> graph(4, 3);
'R[4, 3]( r)'= combine(R(4, 3));
```



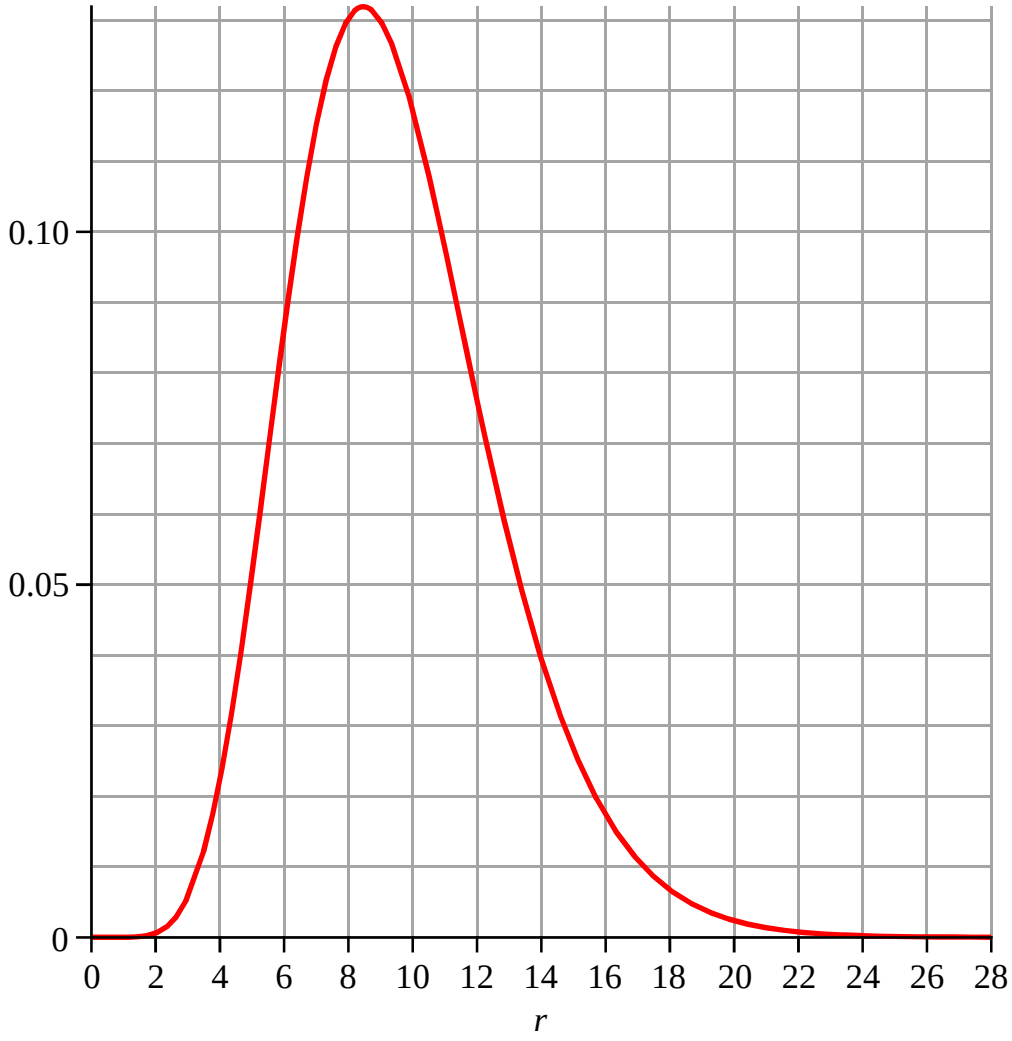
$$R_{4,\,3}(r) = \frac{1}{26880}\,\frac{r^3\sqrt{35}\,\sqrt{\frac{1}{a}}\,e^{-\frac{1}{4}\frac{r}{a}}}{a^4} \qquad \textbf{(28)}$$

> *graphP*(4, 3);

'$r^2 \cdot (\mathrm{abs}(R[4, 3](r)))^2$';

$a := 0.529$:

$'\int_0^{\infty} r^2 |R(4, 3)|^2 \, dr' = \int_0^{\infty} r^2 |R(4, 3)|^2 \, dr$;



$$r^2 \left|R_{4,\,3}(r)\right|^2$$

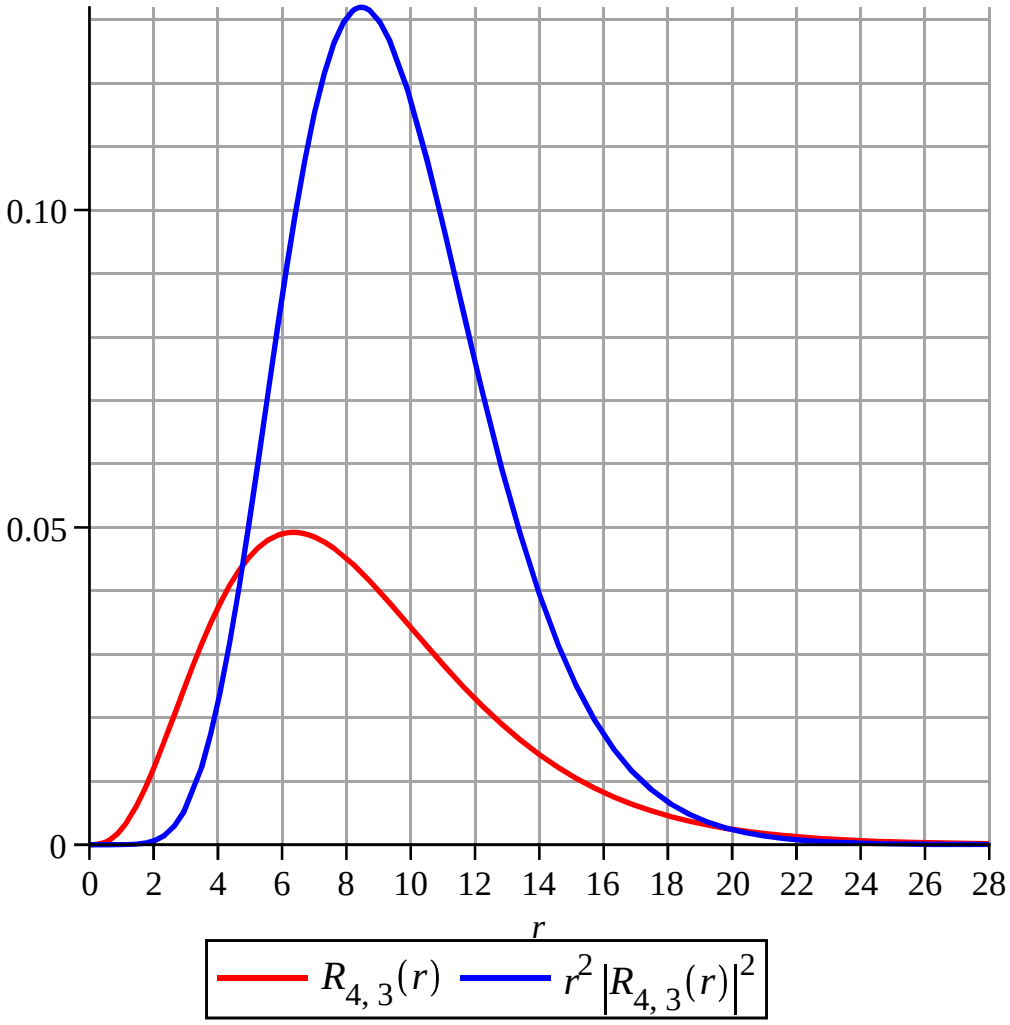
$$\int_0^{\infty} r^2 |R(4, 3)|^2 \, dr = 1.000 \qquad \textbf{(29)}$$

> $r[max] := \max\left(solve\left(\frac{d}{dr}\left(r^2 (R(4, 3))^2\right) = 0\right)\right)$;

$r[max] := 'r[max]'$: $a := 'a'$:

$$r_{max} := 8.464 \qquad \textbf{(30)}$$

```
> graph2(4, 3);
```

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