

$$R21 = \frac{r \operatorname{Exp}\left[-\frac{r}{2aa}\right]}{\sqrt{24} aa^{5/2}}$$

$$\text{Out}[*]:= \frac{e^{-\frac{r}{2a}} r}{2 \sqrt{6} a^{5/2}}$$

$$R20 = \frac{\left(1 - \frac{r}{2a}\right) \operatorname{Exp}\left[-\frac{r}{2aa}\right]}{\sqrt{2} aa^{3/2}}$$

$$\text{Out}[*]:= \frac{e^{-\frac{r}{2a}} \left(1 - \frac{r}{2a}\right)}{\sqrt{2} a^{3/2}}$$

$$\text{In}[*]:= \text{Radial} = (\text{Sqrt}[4 * \text{Pi} / 3]) * \text{Integrate}[r^3 * R21 * R20, \{r, 0, \text{Infinity}\}]$$

$$\text{Out}[*]:= \text{ConditionalExpression}\left[-6 a \sqrt{\pi}, \operatorname{Re}[a] > 0\right]$$

$$\text{In}[*]:= \text{Angular} = 2 \pi \int_0^\pi \text{Conjugate}[\text{SphericalHarmonicY}[0, 0, x, 0]]$$

$$\text{SphericalHarmonicY}[1, 0, x, 0] \text{SphericalHarmonicY}[1, 0, x, 0] \sin[x] dx$$

$$\text{Out}[*]:= \frac{1}{2 \sqrt{\pi}}$$

$$\text{In}[*]:= \text{Radial} * \text{Angular} * (-1 / \text{Sqrt}[3])$$

$$\text{Out}[*]:= \text{ConditionalExpression}\left[\sqrt{3} a, \operatorname{Re}[a] > 0\right]$$

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In[ ]:= Angular1 = 2 \pi \int_0^\pi Conjugate[SphericalHarmonicY[0, 0, x, 0]]
      SphericalHarmonicY[1, -1, x, 0] SphericalHarmonicY[1, 1, x, 0] Sin[x] d x
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$$\text{Out[]} = -\frac{1}{2\sqrt{\pi}}$$

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In[ ]:= Radial * Angular1
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Out[ ] = ConditionalExpression[3 a, Re[a] > 0]
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In[ ]:=
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In[ ]:= R11[a_] = MatrixForm[{{0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, 0, 0}, {0, 0, 0, 0, Sqrt[3] * aa, 0},
      {0, 0, 0, 0, 0, 3 * aa}, {-3 * aa, 0, 0, 0, 0, 0}, {0, -Sqrt[3] * aa, 0, 0, -Sqrt[6] * aa, 0}}]
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Out[ ] //MatrixForm=
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$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{3} aa & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 aa \\ -3 aa & 0 & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{3} aa & 0 & 0 & -\sqrt{6} aa & 0 \end{pmatrix}$$

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In[ ]:= R12[a_] = MatrixForm[{{0, 0, 0, 0, 0, 3 * aa}, {0, 0, 0, 0, 0, \sqrt{3} aa}, {0, 0, 0, 0, 0, 0},
      {0, 0, 0, 0, 0, 0}, {0, 0, -Sqrt[3] * aa, 0, 0, Sqrt[6] * aa}, {0, 0, 0, -3 * aa, 0, 0}}]
```

```
Out[ ] //MatrixForm=
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$$\begin{pmatrix} 0 & 0 & 0 & 0 & 3 aa & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} aa \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{3} aa & 0 & 0 & \sqrt{6} aa \\ 0 & 0 & 0 & -3 aa & 0 & 0 \end{pmatrix}$$

In[]:= X = MatrixForm[

$$(-1/\text{Sqrt}[2]) * \left(\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} aa & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 aa & 0 \\ -3 aa & 0 & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{3} aa & 0 & 0 & -\sqrt{6} aa & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 0 & 3 aa & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} aa \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{3} aa & 0 & 0 & \sqrt{6} aa \\ 0 & 0 & 0 & -3 aa & 0 & 0 \end{pmatrix} \right)$$

Out[]//MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{3 aa}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{\frac{3}{2}} aa \\ 0 & 0 & 0 & 0 & -\sqrt{\frac{3}{2}} aa & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3 aa}{\sqrt{2}} \\ \frac{3 aa}{\sqrt{2}} & 0 & -\sqrt{\frac{3}{2}} aa & 0 & 0 & \sqrt{3} aa \\ 0 & \sqrt{\frac{3}{2}} aa & 0 & -\frac{3 aa}{\sqrt{2}} & \sqrt{3} aa & 0 \end{pmatrix}$$

In[]:= Y = MatrixForm[

$$(I / \text{Sqrt}[2]) * \left(\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} aa & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 aa & 0 \\ -3 aa & 0 & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{3} aa & 0 & 0 & -\sqrt{6} aa & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 3 aa & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} aa \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{3} aa & 0 & 0 & \sqrt{6} aa \\ 0 & 0 & 0 & -3 aa & 0 & 0 \end{pmatrix} \right)$$

Out[]:= MatrixForm=

$$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{3 i aa}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & i \sqrt{\frac{3}{2}} aa \\ 0 & 0 & 0 & 0 & i \sqrt{\frac{3}{2}} aa & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{3 i aa}{\sqrt{2}} \\ -\frac{3 i aa}{\sqrt{2}} & 0 & -i \sqrt{\frac{3}{2}} aa & 0 & 0 & i \sqrt{3} aa \\ 0 & -i \sqrt{\frac{3}{2}} aa & 0 & -\frac{3 i aa}{\sqrt{2}} & -i \sqrt{3} aa & 0 \end{pmatrix}$$

$$\text{In[]:= H13} = 2 \pi e \text{Eext} \sqrt{\frac{4 \pi}{3}} \left(\int_0^\infty r^3 R_{21} R_{20} dr \right) \int_0^\pi \text{Conjugate[SphericalHarmonicY}[0, 0, x, 0]] \\ \text{SphericalHarmonicY}[1, 0, x, 0] \text{SphericalHarmonicY}[1, 0, x, 0] \text{Sin}[x] dx$$

Out[]:= ConditionalExpression[-3 a e Eext, Re[a] > 0]

In[]:= Eigenvalues[{{0, 0, 1, 0}, {0, 0, 0, 0}, {1, 0, 0, 0}, {0, 0, 0, 0}}]

Out[]:= {-1, 1, 0, 0}

$$\text{In}[\circ] := \text{f100}[r_] := \frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}}$$

$$\text{In}[\circ] := \text{f210}[r_ , t_] := \frac{1}{4 \sqrt{2 \pi} a^{3/2}} \frac{r}{a} e^{-\frac{r}{2a}} \cos[t]$$

$$\text{In}[\circ] := \text{f310}[r_ , t_] := \frac{2}{81 \sqrt{\pi} a^{3/2}} \left(6 - \frac{r}{a} \right) \frac{r}{a} e^{-\frac{r}{3a}} \cos[t]$$

$$\text{In}[\circ] := \text{f410}[r_ , t_] := \frac{e^{-\frac{r}{4a}} \sqrt{\frac{5}{\pi}} r \left(1 - \frac{r}{4a} + \frac{r^2}{80a^2} \right) \cos[t]}{32 a^{5/2}}$$

`In[\circ] := ClearAll["Global`*"]`

`F[n_, L_, x_] := x^L E^(-x/2) Factorial[n+L] LaguerreL[n-L-1, 2L+1, x];`

`R[n_, L_, r_] := a^(-3/2) 2/(n^2) Sqrt[Factorial[n-1-L]/(Factorial[n+L])^3]`

`F[n, L, 2r/(na)];`

`H[n_, l_, m_, r_, \theta_, \phi_] = R[n, l, r] * SphericalHarmonicY[l, m, \theta, \phi];`

`H[2, 1, \theta, r, \theta, \phi]`

`a = 5.29 \times 10^{-11}`

$$\text{Out}[\circ] = \frac{\cos[\theta]}{24 a^{3/2} \sqrt{2 \pi}}$$

$$\text{Out}[\circ] = 5.29 \times 10^{-11}$$

$$\text{In}[\circ] := 2 \pi \int_0^\infty \int_0^\pi \frac{1}{4 \sqrt{2 \pi} a^{3/2}} \frac{r}{a} e^{-\frac{r}{2a}} \cos[t] * \frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}} * r \cos[t] (r^2 \sin[t]) dt dr$$

$$\text{Out}[\circ] = 3.94071 \times 10^{-11}$$

`In[\circ] := b = N[%]`

$$\text{Out}[\circ] = 3.94071 \times 10^{-11}$$

$$\text{In}[\text{ }] := 2 \pi \int_0^\infty \int_0^\pi \frac{2}{81 \sqrt{\pi} a^{3/2}} \left(6 - \frac{r}{a} \right) \frac{r}{a} e^{-\frac{r}{3a}} \cos[t] * \frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}} * r \cos[t] (r^2 \sin[t]) dt dr$$

$$\text{Out}[\text{ }] = 2.23172 \times 10^{-11}$$

$$\text{In}[\text{ }] := \mathbf{c} = \mathbf{N}[\%]$$

$$\text{Out}[\text{ }] = 2.23172 \times 10^{-11}$$

$$\text{In}[\text{ }] := 2 \pi \int_0^\infty \int_0^\pi \frac{e^{-\frac{r}{4a}} \sqrt{\frac{5}{\pi}} r \left(1 - \frac{r}{4a} + \frac{r^2}{80a^2} \right) \cos[t]}{32 a^{5/2}} * \frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}} * r \cos[t] (r^2 \sin[t]) dt dr$$

$$\text{Out}[\text{ }] = 9.30255 \times 10^{-12}$$

$$\text{In}[\text{ }] := \mathbf{d} = \mathbf{N}[\%]$$

$$\text{Out}[\text{ }] = 9.30255 \times 10^{-12}$$

$$g[n_] := \frac{-13.6}{n^2}$$

$$n2 = \mathbf{N} \left[\frac{b^2}{g[1] - g[2]} \right]$$

$$\text{Out}[\text{ }] = -1.52247 \times 10^{-22}$$

$$n3 = \mathbf{N} \left[\frac{c^2}{g[1] - g[3]} \right]$$

$$\text{Out}[\text{ }] = -4.11996 \times 10^{-23}$$

$$n4 = \mathbf{N} \left[\frac{d^2}{g[1] - g[4]} \right]$$

$$\text{Out}[\text{ }] = -6.78724 \times 10^{-24}$$

$$\text{In}[\text{ }] := (5.29 \times 10^{\wedge} -11)^{\wedge} 3 * 2.1333333$$

$$\text{Out}[\text{ }] = 3.1581 \times 10^{-31}$$

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In[ ]:= (n2 + n3 + n4) * (1.6 * 10^-19)
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Out[ ]:= -3.20374 × 10-41
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