$$\mathtt{Integrate}\left[\mathtt{Sin}[\theta]\,\mathtt{Cos}[\theta]^2\, r^3\, e^{-2\,r/a},\ \{r,\,0,\,\infty\},\ \{\theta,\,0,\,\pi\},\ \{\phi,\,0,\,2\,\pi\}\right]$$

$$\mathtt{ConditionalExpression}\left[\frac{a^4\,\pi}{2},\ \mathrm{Re}[a] > 0\right]$$

$$\mathtt{Integrate}\left[\mathtt{Sin}[t]^3\,\mathtt{Cos}[t]^2,\ \{t,\,0,\,\pi\}\right]$$

$$\frac{4}{15}$$

$$\mathtt{Integrate}\left[\mathtt{Exp}[-i\,t]\,\mathtt{Cos}[t]^2,\ \{t,\,0,\,2\,\pi\}\right]$$

$$0$$

In[1]:=

$$\begin{aligned}
&H = \mathtt{Table}\Big[\\
&\quad \mathtt{Integrate}\left[i * j * k * r^2\,\mathtt{Sin}[\theta],\ \{r,\,0,\,\infty\},\ \{\theta,\,0,\,\pi\},\ \{\phi,\,0,\,2\,\pi\},\ \mathtt{Assumptions} \to a > 0\right],\\
&\quad \Big\{i,\ \Big\{\frac{1}{4\sqrt{2\,\pi\,a^3}}\left(2-\frac{r}{a}\right)e^{-r/(2\,a)},\ \frac{-1}{8\sqrt{\pi\,a^3}}\left(\frac{r}{a}\right)e^{-r/(2\,a)}\,\mathtt{Sin}[\theta]\,e^{-i\,\phi},\\
&\qquad \frac{1}{4\sqrt{2\,\pi\,a^3}}\left(\frac{r}{a}\right)e^{-r/(2\,a)}\,\mathtt{Cos}[\theta],\ \frac{1}{8\sqrt{\pi\,a^3}}\left(\frac{r}{a}\right)e^{-r/(2\,a)}\,\mathtt{Sin}[\theta]\,e^{i\,\phi}\Big\}\Big\},\\
&\quad \Big\{j,\ \Big\{r^2\,\mathtt{Sin}[\theta]^2\,\mathtt{Cos}[\phi]^2,\ r^2\,\mathtt{Sin}[\theta]^2\,\mathtt{Sin}[\phi]^2,\ r^2\,\mathtt{Cos}[\theta]^2\Big\}\Big\},\\
&\quad \Big\{k,\ \Big\{\frac{1}{4\sqrt{2\,\pi\,a^3}}\left(2-\frac{r}{a}\right)e^{-r/(2\,a)},\ \frac{-1}{8\sqrt{\pi\,a^3}}\left(\frac{r}{a}\right)e^{-r/(2\,a)}\,\mathtt{Sin}[\theta]\,e^{i\,\phi},\\
&\qquad \frac{1}{4\sqrt{2\,\pi\,a^3}}\left(\frac{r}{a}\right)e^{-r/(2\,a)}\,\mathtt{Cos}[\theta],\ \frac{1}{8\sqrt{\pi\,a^3}}\left(\frac{r}{a}\right)e^{-r/(2\,a)}\,\mathtt{Sin}[\theta]\,e^{-i\,\phi}\Big\}\Big\}\Big]\ \mathtt{//\ MatrixForm}
\end{aligned}$$

Out[1]//MatrixForm=

$$\begin{pmatrix}
\begin{pmatrix}14\,a^2\\0\\0\\0\end{pmatrix} & \begin{pmatrix}14\,a^2\\0\\0\\0\end{pmatrix} & \begin{pmatrix}14\,a^2\\0\\0\\0\end{pmatrix}\\
\begin{pmatrix}0\\12\,a^2\\0\\-6\,a^2\end{pmatrix} & \begin{pmatrix}0\\12\,a^2\\0\\6\,a^2\end{pmatrix} & \begin{pmatrix}0\\6\,a^2\\0\\0\end{pmatrix}\\
\begin{pmatrix}0\\0\\6\,a^2\\0\end{pmatrix} & \begin{pmatrix}0\\0\\6\,a^2\\0\end{pmatrix} & \begin{pmatrix}0\\0\\18\,a^2\\0\end{pmatrix}\\
\begin{pmatrix}0\\-6\,a^2\\0\\12\,a^2\end{pmatrix} & \begin{pmatrix}0\\6\,a^2\\0\\12\,a^2\end{pmatrix} & \begin{pmatrix}0\\0\\0\\6\,a^2\end{pmatrix}
\end{pmatrix}$$

```
Table[{i, j, k}, {i, {i1, i2, i3, i4}},
  {j, {j1, j2, j3}}, {k, {k1, k2, k3, k4}}] // MatrixForm
```

$$\begin{pmatrix} \begin{pmatrix} i1 & j1 & k1 \\ i1 & j1 & k2 \\ i1 & j1 & k3 \\ i1 & j1 & k4 \end{pmatrix} & \begin{pmatrix} i1 & j2 & k1 \\ i1 & j2 & k2 \\ i1 & j2 & k3 \\ i1 & j2 & k4 \end{pmatrix} & \begin{pmatrix} i1 & j3 & k1 \\ i1 & j3 & k2 \\ i1 & j3 & k3 \\ i1 & j3 & k4 \end{pmatrix} \\ \begin{pmatrix} i2 & j1 & k1 \\ i2 & j1 & k2 \\ i2 & j1 & k3 \\ i2 & j1 & k4 \end{pmatrix} & \begin{pmatrix} i2 & j2 & k1 \\ i2 & j2 & k2 \\ i2 & j2 & k3 \\ i2 & j2 & k4 \end{pmatrix} & \begin{pmatrix} i2 & j3 & k1 \\ i2 & j3 & k2 \\ i2 & j3 & k3 \\ i2 & j3 & k4 \end{pmatrix} \\ \begin{pmatrix} i3 & j1 & k1 \\ i3 & j1 & k2 \\ i3 & j1 & k3 \\ i3 & j1 & k4 \end{pmatrix} & \begin{pmatrix} i3 & j2 & k1 \\ i3 & j2 & k2 \\ i3 & j2 & k3 \\ i3 & j2 & k4 \end{pmatrix} & \begin{pmatrix} i3 & j3 & k1 \\ i3 & j3 & k2 \\ i3 & j3 & k3 \\ i3 & j3 & k4 \end{pmatrix} \\ \begin{pmatrix} i4 & j1 & k1 \\ i4 & j1 & k2 \\ i4 & j1 & k3 \\ i4 & j1 & k4 \end{pmatrix} & \begin{pmatrix} i4 & j2 & k1 \\ i4 & j2 & k2 \\ i4 & j2 & k3 \\ i4 & j2 & k4 \end{pmatrix} & \begin{pmatrix} i4 & j3 & k1 \\ i4 & j3 & k2 \\ i4 & j3 & k3 \\ i4 & j3 & k4 \end{pmatrix} \end{pmatrix}$$

```
In[28]:= Hx = {H[[1]][[1]][[1]], H[[1]][[2]][[1]], H[[1]][[3]][[1]], H[[1]][[4]][[1]]};
         Hy = {H[[1]][[1]][[2]], H[[1]][[2]][[2]], H[[1]][[3]][[2]], H[[1]][[4]][[2]]};
         Hz = {H[[1]][[1]][[3]], H[[1]][[2]][[3]], H[[1]][[3]][[3]], H[[1]][[4]][[3]]};

In[31]:= Hx // MatrixForm
```

Out[31]//MatrixForm=

$$\begin{pmatrix} 14\,a^2 & 0 & 0 & 0 \\ 0 & 12\,a^2 & 0 & -6\,a^2 \\ 0 & 0 & 6\,a^2 & 0 \\ 0 & -6\,a^2 & 0 & 12\,a^2 \end{pmatrix}$$

```
In[32]:= Hy // MatrixForm
```

Out[32]//MatrixForm=

$$\begin{pmatrix} 14\,a^2 & 0 & 0 & 0 \\ 0 & 12\,a^2 & 0 & 6\,a^2 \\ 0 & 0 & 6\,a^2 & 0 \\ 0 & 6\,a^2 & 0 & 12\,a^2 \end{pmatrix}$$

```
In[33]:= Hz // MatrixForm
```

Out[33]//MatrixForm=

$$\begin{pmatrix} 14\,a^2 & 0 & 0 & 0 \\ 0 & 6\,a^2 & 0 & 0 \\ 0 & 0 & 18\,a^2 & 0 \\ 0 & 0 & 0 & 6\,a^2 \end{pmatrix}$$

$$\begin{aligned} \left\langle i \middle| H' \middle| j \right\rangle &= \left\langle i \middle| V_0 + 3(\beta_1 x^2 + \beta_2 y^2 + \beta_3 z^2) - (\beta_1+\beta_2+\beta_3) r^2 \middle| j \right\rangle = \\ &\left\langle i \middle| V_0 \middle| j \right\rangle + \left\langle i \middle| 3(\beta_1 x^2 + \beta_2 y^2 + \beta_3 z^2) \middle| j \right\rangle + \left\langle i \middle| -(\beta_1+\beta_2+\beta_3) r^2 \middle| j \right\rangle \\ &= \left\langle i \middle| V_0 \middle| j \right\rangle + 3\beta_1 \left\langle i \middle| x^2 \middle| j \right\rangle + 3\beta_2 \left\langle i \middle| y^2 \middle| j \right\rangle + 3\beta_3 \left\langle i \middle| z^2 \middle| j \right\rangle - (\beta_1+\beta_2+\beta_3) \left\langle i \middle| r^2 \middle| j \right\rangle \\ &= V_0 \boldsymbol{I} + 3\beta_1 \mathbf{Hx} + 3\beta_2 \mathbf{Hy} + 3\beta_3 \mathbf{Hz} - (\beta_1+\beta_2+\beta_3)(\mathbf{Hx}+\mathbf{Hy}+\mathbf{Hz}) \end{aligned}$$

```
In[36]:= representationH = V0 IdentityMatrix[4] + 2 β1 Hx + 2 β2 Hy + 2 β3 Hz
```

Out[36]=

$$\{\{V_0 + 28\,a^2\,\beta_1 + 28\,a^2\,\beta_2 + 28\,a^2\,\beta_3,\ 0,\ 0,\ 0\},$$
$$\{0,\ V_0 + 24\,a^2\,\beta_1 + 24\,a^2\,\beta_2 + 12\,a^2\,\beta_3,\ 0,\ -12\,a^2\,\beta_1 + 12\,a^2\,\beta_2\},$$
$$\{0,\ 0,\ V_0 + 12\,a^2\,\beta_1 + 12\,a^2\,\beta_2 + 36\,a^2\,\beta_3,\ 0\},$$
$$\{0,\ -12\,a^2\,\beta_1 + 12\,a^2\,\beta_2,\ 0,\ V_0 + 24\,a^2\,\beta_1 + 24\,a^2\,\beta_2 + 12\,a^2\,\beta_3\}\}$$

In[37]:= **representationH // MatrixForm**

Out[37]//MatrixForm=

$$\begin{pmatrix} V_0 + 28\,a^2\,\beta_1 + 28\,a^2\,\beta_2 + 28\,a^2\,\beta_3 & 0 & 0 & \\ 0 & V_0 + 24\,a^2\,\beta_1 + 24\,a^2\,\beta_2 + 12\,a^2\,\beta_3 & 0 & \\ 0 & 0 & V_0 + 12\,a^2\,\beta_1 + 12\,a^2\,\beta_2 + 36\,a^2\,\beta_3 & \\ 0 & -12\,a^2\,\beta_1 + 12\,a^2\,\beta_2 & 0 & V \end{pmatrix}$$

In[38]:= **Eigenvalues[%37]**

Out[38]= $\{V_0 + 36\,a^2\,\beta_1 + 12\,a^2\,\beta_2 + 12\,a^2\,\beta_3,\ V_0 + 12\,a^2\,\beta_1 + 36\,a^2\,\beta_2 + 12\,a^2\,\beta_3,$
$V_0 + 28\,a^2\,\beta_1 + 28\,a^2\,\beta_2 + 28\,a^2\,\beta_3,\ V_0 + 12\,a^2\,\beta_1 + 12\,a^2\,\beta_2 + 36\,a^2\,\beta_3\}$