In[14]:=
$$\psi[n\_, l\_, m\_, r\_, \theta\_, \varphi\_] := \sqrt{\frac{8\,(n-l-1)!}{(n\,a_0)^3\,2n\,(n+l)!}}\; e^{-\frac{r}{n a_0}} \left(\frac{2r}{n a_0}\right)^l \text{LaguerreL}\left[n-l-1,\, 2l+1,\, \frac{2r}{n a_0}\right] \text{SphericalHarmonicY}[l, m, \theta, \varphi]$$

In[15]:=
```
States = {ψ[2, 0, 0, r, θ, φ], ψ[2, 1, -1, r, θ, φ], ψ[2, 1, 0, r, θ, φ], ψ[2, 1, 1, r, θ, φ]};
```

In[16]:=
```
M = Table[Simplify[Integrate[Conjugate[States[[i]]] States[[j]] r^2 Sin[θ]^2 Cos[φ] Sin[φ],
      {r, 0, ∞}, {θ, 0, π}, {φ, 0, 2 π}], a0 > 0], {i, 4}, {j, 4}] // MatrixForm
```

Out[16]//MatrixForm=
$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{9\,i\,\pi}{128} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{9\,i\,\pi}{128} & 0 & 0 \end{pmatrix}$$