In[1]:= **f = Table@D@Exp@- b r^2D, 8b, n<D, 8n, 0, 3<D**

Out[1]= $9\tilde{a}^{-b r^2}, -\tilde{a}^{-b r^2} r^2, \tilde{a}^{-b r^2} r^4, -\tilde{a}^{-b r^2} r^6=$

In[2]:= **ff@r_, n_D = $\tilde{a}^{-b r^2}$ H-1L^n r^H2 nL**

Out[2]= $H\text{-}1L^n \tilde{a}^{-b r^2} r^{2n}$

In[3]:= **H* Overlap matrix *L**

In[4]:= **s = Table@**
HIntegrate@H4 Pi r^2 ff@r, mD ff@r, nDL , 8r, 0, Infinity<D •• Simplify@#, Re@bD > 0D &L,
8m, 1, 4<, 8n, 1, 4<D

Out[4]= $::\frac{15\, p^{3\bullet2}}{32\sqrt{2}\, b^{7\bullet2}}, -\frac{105\, p^{3\bullet2}}{128\sqrt{2}\, b^{9\bullet2}}, \frac{945\, p^{3\bullet2}}{512\sqrt{2}\, b^{11\bullet2}}, -\frac{10395\, p^{3\bullet2}}{2048\sqrt{2}\, b^{13\bullet2}}>,$

$:-\frac{105\, p^{3\bullet2}}{128\sqrt{2}\, b^{9\bullet2}}, \frac{945\, p^{3\bullet2}}{512\sqrt{2}\, b^{11\bullet2}}, -\frac{10395\, p^{3\bullet2}}{2048\sqrt{2}\, b^{13\bullet2}}, \frac{135135\, p^{3\bullet2}}{8192\sqrt{2}\, b^{15\bullet2}}>,$

$:\frac{945\, p^{3\bullet2}}{512\sqrt{2}\, b^{11\bullet2}}, -\frac{10395\, p^{3\bullet2}}{2048\sqrt{2}\, b^{13\bullet2}}, \frac{135135\, p^{3\bullet2}}{8192\sqrt{2}\, b^{15\bullet2}}, -\frac{2027025\, p^{3\bullet2}}{32768\sqrt{2}\, b^{17\bullet2}}>,$

$:-\frac{10395\, p^{3\bullet2}}{2048\sqrt{2}\, b^{13\bullet2}}, \frac{135135\, p^{3\bullet2}}{8192\sqrt{2}\, b^{15\bullet2}}, -\frac{2027025\, p^{3\bullet2}}{32768\sqrt{2}\, b^{17\bullet2}}, \frac{34459425\, p^{3\bullet2}}{131072\sqrt{2}\, b^{19\bullet2}}>>$

In[5]:= **H* Here is the general formula for the overlap *L**

In[6]:= **Integrate@H4 Pi r^2 ff@r, mD ff@r, nDL , 8r, 0, Infinity<D ••**
Simplify@#, 8Re@bD > 0, n >= 0, m >= 0, n Î Integers, m Î Integers<D &

Out[6]= $H\text{-}1L^{m+n}\, 2^{-\frac{1}{2}-m-n}\, b^{-\frac{3}{2}-m-n}\, p\ \text{GammaA}\frac{3}{2} + m + n\text{E}$

In[7]:= **%6 •. m ® 1 •. n ® 1**

Out[7]= $\frac{15\, p^{3\bullet2}}{32\sqrt{2}\, b^{7\bullet2}}$

In[8]:= **TableForm[s]**

Out[8]//TableForm=

$\frac{15\pi^{3/2}}{32\sqrt{2}\,b^{7/2}}$	$-\frac{105\pi^{3/2}}{128\sqrt{2}\,b^{9/2}}$	$\frac{945\pi^{3/2}}{512\sqrt{2}\,b^{11/2}}$	$-\frac{10395\pi^{3/2}}{2048\sqrt{2}\,b^{13/2}}$
$-\frac{105\pi^{3/2}}{128\sqrt{2}\,b^{9/2}}$	$\frac{945\pi^{3/2}}{512\sqrt{2}\,b^{11/2}}$	$-\frac{10395\pi^{3/2}}{2048\sqrt{2}\,b^{13/2}}$	$\frac{135135\pi^{3/2}}{8192\sqrt{2}\,b^{15/2}}$
$\frac{945\pi^{3/2}}{512\sqrt{2}\,b^{11/2}}$	$-\frac{10395\pi^{3/2}}{2048\sqrt{2}\,b^{13/2}}$	$\frac{135135\pi^{3/2}}{8192\sqrt{2}\,b^{15/2}}$	$-\frac{2027025\pi^{3/2}}{32768\sqrt{2}\,b^{17/2}}$
$-\frac{10395\pi^{3/2}}{2048\sqrt{2}\,b^{13/2}}$	$\frac{135135\pi^{3/2}}{8192\sqrt{2}\,b^{15/2}}$	$-\frac{2027025\pi^{3/2}}{32768\sqrt{2}\,b^{17/2}}$	$\frac{34459425\pi^{3/2}}{131072\sqrt{2}\,b^{19/2}}$

In[9]:= **(* Laplacian in Spherical Coordinates *)**

In[10]:= **<< Calculus`VectorAnalysis`**

In[11]:= **(* Function of r only (i.e. spherically symmetric *)**

In[12]:= **Laplacian[g[r], Spherical[r, theta, phi]]**

General::spell1 : Possible spelling error: new symbol name "theta" is similar to existing symbol "Ttheta".

Out[12]= $\frac{\mathrm{Csc}[theta]\,(2\,r\,\mathrm{Sin}[theta]\,g'[r] + r^2\,\mathrm{Sin}[theta]\,g''[r])}{r^2}$

In[13]:= **TrigExpand[%]**

Out[13]= $\frac{2\,r\,g'[r] + r^2\,g''[r]}{r^2}$

In[14]:= **(* Hamiltonian in spherical coordinates *)**

In[15]:= **hamiltonian[V_][psi_] := -(1/2) (2 r D[psi, r] + r^2 D[psi, {r, 2}])/r^2 + V psi**

In[16]:= **(* We get 4 Pi from the integration theta and phi, and r^2 also from the Jacobian of the transformation from cartseian to spherical coordinates *)**

In[17]:= **hh = Integrate[(4 Pi r^2 ff[r, m] hamiltonian[1/r][ff[r, n]]), {r, 0, Infinity}] // Simplify[#, {Re[b] > 0, n >= 0, m >= 0, n ∈ Integers, m ∈ Integers}] &**

Out[17]= $(-1)^{m+n}\, 2^{-\frac{1}{2}-m-n}\, b^{-1-m-n}\, \pi \left(-2\sqrt{b}\, n\,(1+2n)\,\mathrm{Gamma}\left[\frac{1}{2}+m+n\right] + \sqrt{2}\,\mathrm{Gamma}[1+m+n] + \sqrt{b}\left((3+4n)\,\mathrm{Gamma}\left[\frac{3}{2}+m+n\right] - \mathrm{Gamma}\left[\frac{5}{2}+m+n\right]\right)\right)$

In[18]:= **hh = FullSimplify[hh, {Re[b] > 0, n >= 0, m >= 0, n ∈ Integers, m ∈ Integers}]**

Out[18]= $(-1)^{m+n}\, 2^{-\frac{1}{2}-m-n}\, b^{-1-m-n}\, \pi \left(\sqrt{2}\,(m+n)! + \sqrt{b}\left(-2\,n\,(1+2n)\,\mathrm{Gamma}\left[\frac{1}{2}+m+n\right] + (3+4n)\,\mathrm{Gamma}\left[\frac{3}{2}+m+n\right] - \mathrm{Gamma}\left[\frac{5}{2}+m+n\right]\right)\right)$

In[19]:= **FortranForm@%D**

Out[19]//FortranForm=

```
          (-1)**(m + n)*2**(-0.5 - m - n)*b**(-1 - m - n)*Pi*
        -  (Sqrt(2)*Factorial(m + n) + Sqrt(b)*(-2*n*(1 + 2*n)*Gamma(0.5 + m + n) + (3 +
   4*n)*Gamma(1.5 + m + n) - Gamma(2.5 + m + n)))
```

In[20]:= **H* Here is a table for hmn *L**

In[21]:= **h = Table@HIntegrate@H r^2 f@@mDD hamiltonian@1 • rD ž f@@nDDL , 8r, 0, Infinity<D •• Simplify@#, Re@bD > 0D &L, 8m, 1, 4<, 8n, 1, 4<D**

Out[21]=

$$\left\{\left\{\frac{8+3\sqrt{b}\sqrt{2\pi}}{32\,b},\ -\frac{16+3\sqrt{b}\sqrt{2\pi}}{128\,b^2},\ \frac{64-15\sqrt{b}\sqrt{2\pi}}{512\,b^3},\ \frac{3\left(-128+105\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4}\right\},\right.$$
$$\left\{-\frac{16+3\sqrt{b}\sqrt{2\pi}}{128\,b^2},\ \frac{64+33\sqrt{b}\sqrt{2\pi}}{512\,b^3},\ -\frac{3\left(128+55\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4},\ \frac{3072+315\sqrt{b}\sqrt{2\pi}}{8192\,b^5}\right\},$$
$$\left\{\frac{64-15\sqrt{b}\sqrt{2\pi}}{512\,b^3},\ -\frac{3\left(128+55\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4},\ \frac{3072+1995\sqrt{b}\sqrt{2\pi}}{8192\,b^5},\right.$$
$$\left.-\frac{15\left(2048+1197\sqrt{b}\sqrt{2\pi}\right)}{32768\,b^6}\right\},\ \left\{\frac{3\left(-128+105\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4},\ \frac{3072+315\sqrt{b}\sqrt{2\pi}}{8192\,b^5},$$
$$\left.\left.-\frac{15\left(2048+1197\sqrt{b}\sqrt{2\pi}\right)}{32768\,b^6},\ \frac{45\left(8192+6237\sqrt{b}\sqrt{2\pi}\right)}{131072\,b^7}\right\}\right\}$$

In[22]:= **TableForm@%D**

Out[22]//TableForm=

$\frac{8+3\sqrt{b}\sqrt{2\pi}}{32\,b}$	$-\frac{16+3\sqrt{b}\sqrt{2\pi}}{128\,b^2}$	$\frac{64-15\sqrt{b}\sqrt{2\pi}}{512\,b^3}$	$\frac{3\left(-128+105\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4}$
$-\frac{16+3\sqrt{b}\sqrt{2\pi}}{128\,b^2}$	$\frac{64+33\sqrt{b}\sqrt{2\pi}}{512\,b^3}$	$-\frac{3\left(128+55\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4}$	$\frac{3072+315\sqrt{b}\sqrt{2\pi}}{8192\,b^5}$
$\frac{64-15\sqrt{b}\sqrt{2\pi}}{512\,b^3}$	$-\frac{3\left(128+55\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4}$	$\frac{3072+1995\sqrt{b}\sqrt{2\pi}}{8192\,b^5}$	$-\frac{15\left(2048+1197\sqrt{b}\sqrt{2\pi}\right)}{32768\,b^6}$
$\frac{3\left(-128+105\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^4}$	$\frac{3072+315\sqrt{b}\sqrt{2\pi}}{8192\,b^5}$	$-\frac{15\left(2048+1197\sqrt{b}\sqrt{2\pi}\right)}{32768\,b^6}$	$\frac{45\left(8192+6237\sqrt{b}\sqrt{2\pi}\right)}{131072\,b^7}$

In[23]:= **H* Here is a check that the formula gives the same result as the table *L**

In[24]:= **hh •. m ® 3 •. n ® 1 •• N •• Factor**

Out[24]=

$$\frac{1.211212679\left(3.890637096+1.\sqrt{b}\right)}{b^5}$$

In[25]:= $\frac{3\pi\left(1024+105\sqrt{b}\sqrt{2\pi}\right)}{2048\,b^5}$ **•• N •• Factor**

Out[25]=

$$\frac{1.211212679\left(3.890637096+1.\sqrt{b}\right)}{b^5}$$