In[∘]:=
```
SetOptions[SelectedNotebook[],
  PrintingStyleEnvironment → "Printout", ShowSyntaxStyles → True]
```

In[∘]:=
```
<< Notation`
```

In[∘]:=
```
Notation[ x_n_ ⟺ x_〚n_〛 ]
```

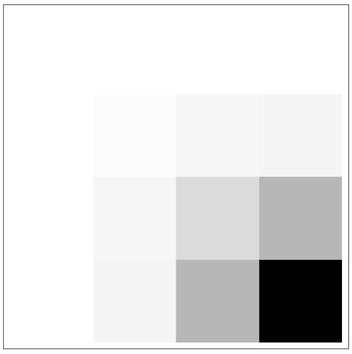
In[∘]:=
```
χ[α_?NumericQ] := Exp[-α r^2]; (* Basis function *)
α = {13.00773, 1.962079, 0.444529, 0.1219492};
(* Coefficients for the basis expansion *)
```

In[∘]:=

$$S = \text{Array}\left[\left(\frac{\pi}{\alpha_{\#1} + \alpha_{\#2}}\right)^{\frac{3}{2}} \&, \{4, 4\}\right]; \text{(* Overlap matrix *)}$$

```
#[S] & /@ {SymmetricMatrixQ, ArrayPlot, MatrixForm}
```

Out[∘]=

{True, ,

$$\begin{pmatrix} 0.0419641 & 0.0961392 & 0.112858 & 0.117043 \\ 0.0961392 & 0.716317 & 1.49148 & 1.85084 \\ 0.112858 & 1.49148 & 6.64247 & 13.0602 \\ 0.117043 & 1.85084 & 13.0602 & 46.2287 \end{pmatrix}$$

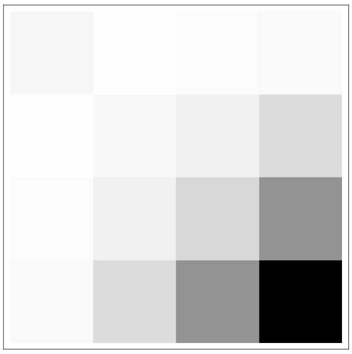
}

In[∘]:=

$$H = \text{Array}\left[\frac{3\,\pi^{3/2}\,\alpha_{\#1}\,\alpha_{\#2}}{(\alpha_{\#1} + \alpha_{\#2})^{5/2}} - \frac{2\,\pi}{\alpha_{\#1} + \alpha_{\#2}} \&, \{4, 4\}\right]; \text{(* Hamiltonian matrix *)}$$

```
#[H] & /@ {SymmetricMatrixQ, ArrayPlot, MatrixForm}
```

Out[∘]=

{True, ,

$$\begin{pmatrix} 0.577268 & 0.0720025 & -0.32154 & -0.436126 \\ 0.0720025 & 0.50705 & -0.989185 & -2.37742 \\ -0.32154 & -0.989185 & -2.63808 & -7.34222 \\ -0.436126 & -2.37742 & -7.34222 & -17.3052 \end{pmatrix}$$

}

```
{evals, evecs} = Eigensystem[{H, S}]; (* Eigenvalues and eigenvectors *)
evals
```

Out[∘]=

```
{21.1444, 2.5923, -0.499278, 0.113214}
```

```
gdEval = Min@evals Eh (* Ground-state eigenvalue *)
UnitConvert[gdEval, "Electronvolts"]
PercentForm@Abs[(gdEval - -13.6058 eV)/(-13.6058 eV)]
 (* Percent error on the reference value *)
```

Out[ ]=

$-0.499278\,E_h$

Out[ ]=

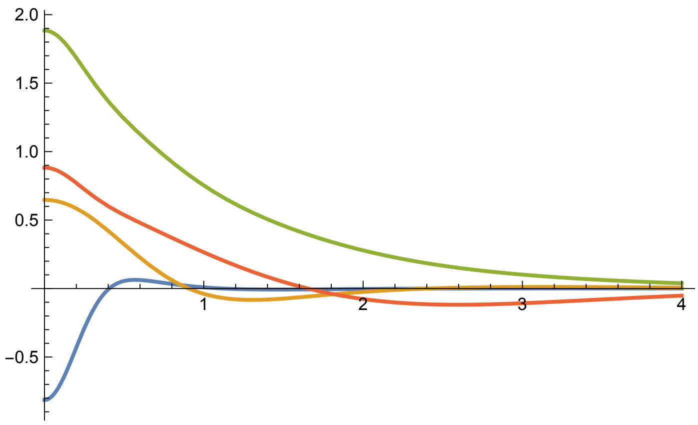
$-13.5861\ \mathrm{eV}$

Out[ ]//PercentForm=

0.1451%

```
efns = #.Array[χ[α#] &, {4}] & /@ evecs;
Plot[efns, {r, 0, 4}, PlotRange → All]
```

Out[ ]=




```
gdTruth = Sqrt[1/π] Exp[-r]; (* Ground truth gdTruth for the comparison *)

(* Out of all the elements of the list efns
 select the one which has the maximum integral *)
filter = Select[efns, NIntegrate[Abs[#]^2, {r, 0, ∞}] ==
      Max[NIntegrate[Abs[#]^2, {r, 0, ∞}] & /@ efns] &] // First;
(* Calculate the normalization for such function *)
expCalc = NIntegrate[4 π r^2 Abs[filter]^2, {r, 0, ∞}];
res = filter/Sqrt[expCalc] // Simplify
```

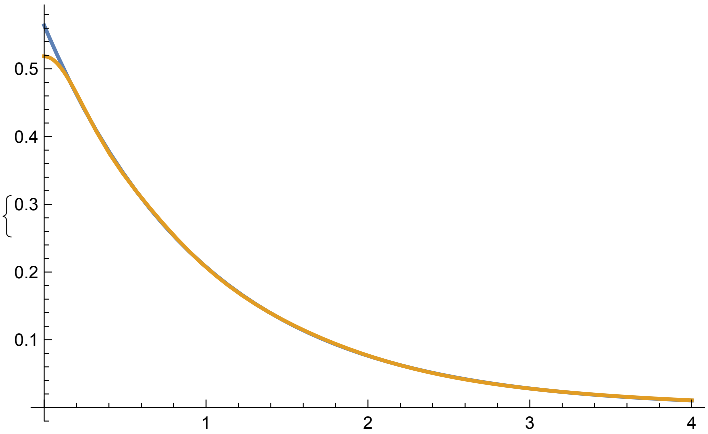
Out[ ]=

$$0.0961015\,e^{-13.0077\,r^2} + 0.163017\,e^{-1.96208\,r^2} + 0.185587\,e^{-0.444529\,r^2} + 0.0737008\,e^{-0.121949\,r^2}$$

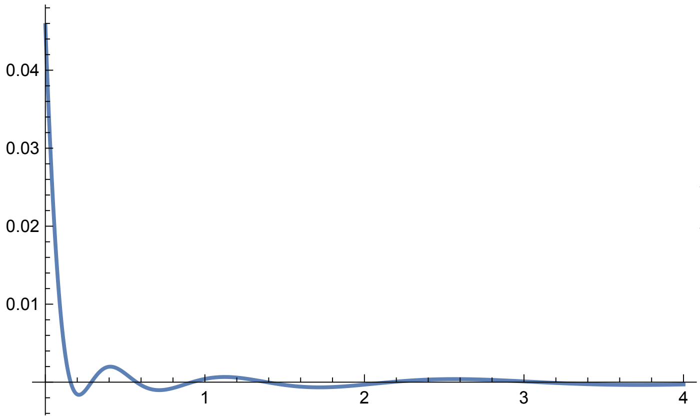
```
(* Plot of the solution obtained with
 the BO method compared to the theoretical one,
on the side there is the plot of the difference of the functions *)
Plot[#, {r, 0, 4}, PlotRange → Full, ImageSize → Medium] & /@
 {{gdTruth, res}, gdTruth - res}
```

Out[ ] =

{




,




}

```
gdTruth - res /. {r → 0} (* The maximum difference between
  the BO approximation with 4 orbitals and the ground truth *)
```

Out[ ] =

```
0.0457831
```