In[54]:=
```
SetOptions[SelectedNotebook[],
 PrintingStyleEnvironment → "Printout", ShowSyntaxStyles → True]
```

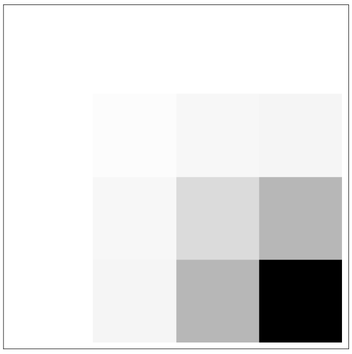
In[55]:=
```
<< Notation`
```

In[56]:=
```
Notation[ x_n_ ⟺ x_[[n_]] ]
```

In[57]:=
```
χ[α_?NumericQ] := Exp[-α r^2]; (* Basis function *)
α = {13.00773, 1.962079, 0.444529, 0.1219492};
(* Coefficients for the basis expansion *)
```

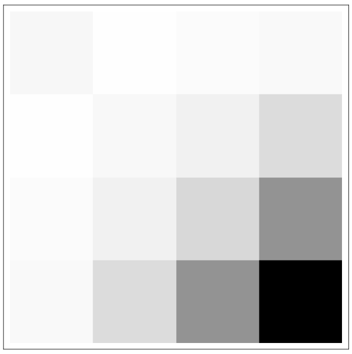
In[59]:=
```
S = Array[(π/(α_#1 + α_#2))^(3/2) &, {4, 4}]; (* Overlap matrix *)
#[S] & /@ {SymmetricMatrixQ, ArrayPlot, MatrixForm}
```

Out[60]=

{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[61]:=
```
H = Array[(3 π^(3/2) α_#1 α_#2)/(α_#1 + α_#2)^(5/2) - (2 π)/(α_#1 + α_#2) &, {4, 4}]; (* Hamiltonian matrix *)
#[H] & /@ {SymmetricMatrixQ, ArrayPlot, MatrixForm}
```

Out[62]=

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

In[63]:=
```
{λ, ψ} = Eigensystem[{H, S}]; (* Eigenvalues and eigenvectors *)
λ
```

Out[64]=

{21.1444, 2.5923, -0.499278, 0.113214}

In[65]:=
```
ϵ = Min@λ E_h (* Ground-state eigenvalue *)
UnitConvert[ϵ, "Electronvolts"]
PercentForm@Abs[(ϵ - -13.6058 eV)/(-13.6058 eV)] (* Percent error on the reference value *)
```

Out[65]=

```
-0.499278 E_h
```

Out[66]=

```
-13.5861 eV
```

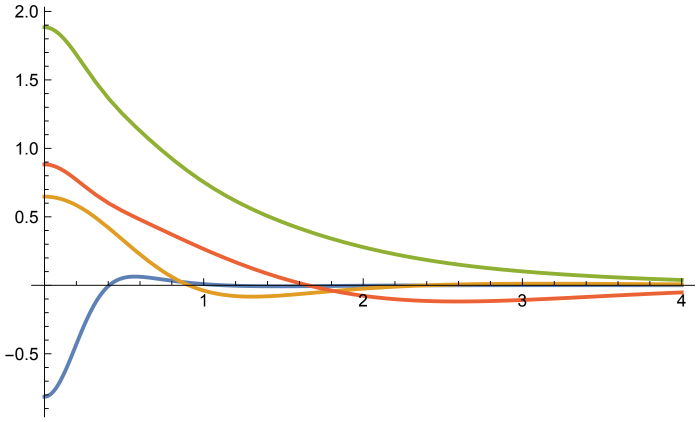
Out[67]//PercentForm=

```
0.1451%
```

In[68]:=

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

Out[69]=



In[70]:=

$$\gamma = \sqrt{\frac{1}{\pi}}\ \text{Exp}[-r];\ \text{(* Ground truth } \gamma \text{ for the comparison *)}$$

In[71]:=

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

$$\theta = \frac{\phi}{\sqrt{\eta}}\ \text{// Simplify}$$

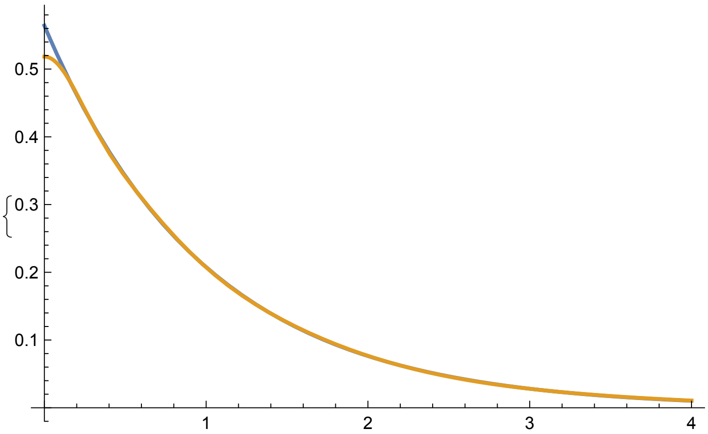
Out[73]=

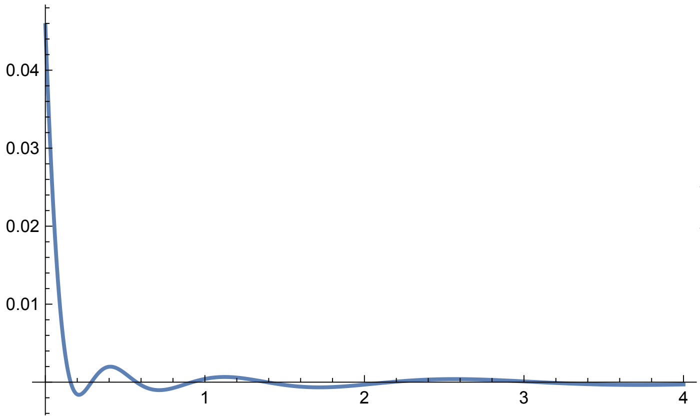
$$0.0961015\, e^{-13.0077\, r^2} + 0.163017\, e^{-1.96208\, r^2} + 0.185587\, e^{-0.444529\, r^2} + 0.0737008\, e^{-0.121949\, r^2}$$

In[74]:=

```
(* 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] & /@ {{γ, θ}, γ - θ}
```

Out[74]=

{,

}


```
In[75]:= γ - θ /. {r → 0} (* The maximum difference between the
  BO approximation with 4 orbitals and the ground truth *)
```

Out[75]=

0.0457831