In[305]:=

```
SetOptions[SelectedNotebook[],
 PrintingStyleEnvironment → "Printout", ShowSyntaxStyles → True]
```

In[306]:=

```
<< Notation`
```

In[307]:=

```
(* Simplify the notation for the
 formulas: index vectors based on a subscript notation *)
Notation[ x_n_ ⟺ x_[[n_]] ]
```

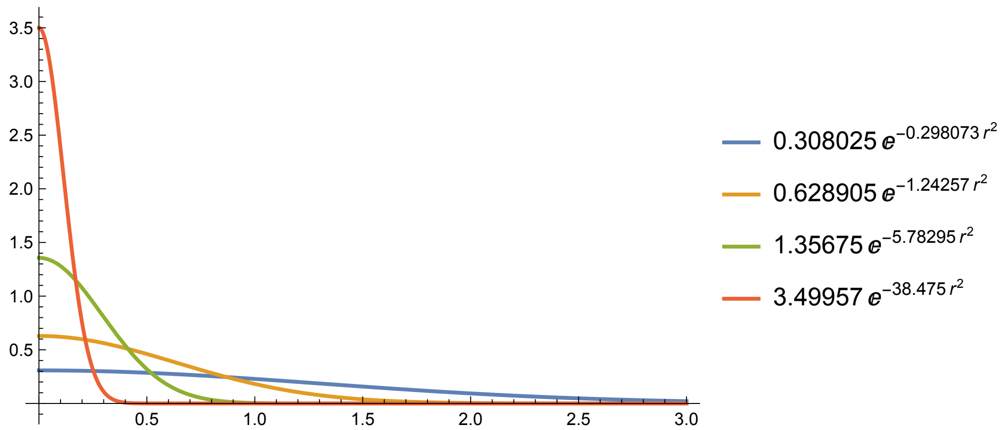
In[308]:=

```
χ[α_?NumericQ] := Exp[-α r^2] Sqrt[α/π];
α = {0.298073, 1.242567, 5.782948, 38.474970};
```

In[310]:=

```
With[{X = Array[χ[α_#] &, {4}]},
 Plot[X, {r, 0, 3}, PlotLegends → "Expressions", PlotRange → All]]
```

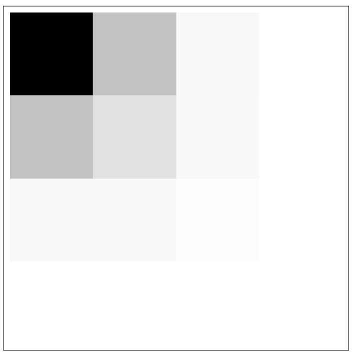
Out[310]=



In[311]:=

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

Out[312]=

{True,  , $\begin{pmatrix} 12.0975 & 2.91188 & 0.37133 & 0.0230638 \\ 2.91188 & 1.42135 & 0.299025 & 0.022246 \\ 0.37133 & 0.299025 & 0.141565 & 0.018912 \\ 0.0230638 & 0.022246 & 0.018912 & 0.00824921 \end{pmatrix}$ }

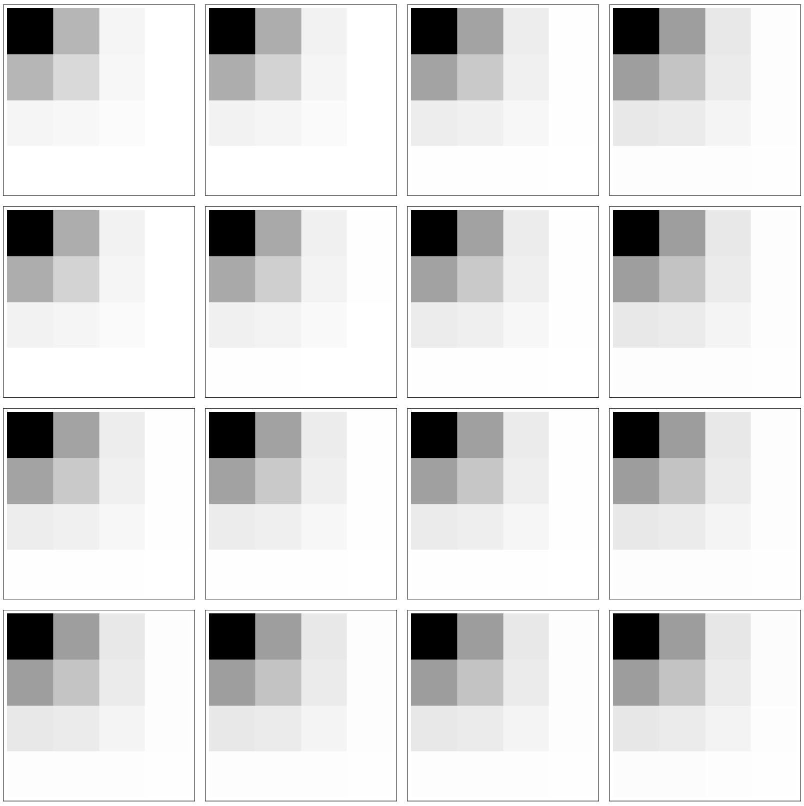
In[313]:=

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

```
{SymmetricMatrixQ[Q],
 Grid@Array[ArrayPlot[Q[[#1,#2]], ImageSize → Tiny] &, {4, 4}], MatrixForm@Q}
```

Out[314]=

{False,



,

90.1588	26
26.0598	13
3.7349	3.
0.241237	0.2
26.0598	8.3
8.39724	4.5
1.3527	1.1
0.092246	0.08
3.7349	1.
1.3527	0.7
0.271299	0.2
0.0221563	0.0
0.241237	0.0
0.092246	0.05
0.0221563	0.01
0.0026428	0.00

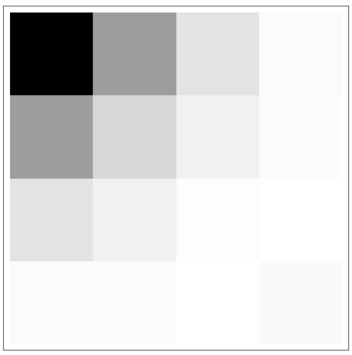
In[315]:=

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

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

Out[316]=

{True,



,

$$\begin{pmatrix} -15.6704 & -6.05651 & -1.75072 & -0.303635 \\ -6.05651 & -2.40744 & -0.871147 & -0.236062 \\ -1.75072 & -0.871147 & 0.141492 & 0.00129568 \\ -0.303635 & -0.236062 & 0.00129568 & 0.312776 \end{pmatrix}$$

}

In[317]:=

$$\text{MatrixNormalize}[v\_,\ M\_] := \frac{v}{\text{Sqrt}[v.M.v]}$$

In[318]:=

```
B = MatrixNormalize[ConstantArray[2., {4}], S]
B.S.B
```

Out[318]=

```
{0.218418, 0.218418, 0.218418, 0.218418}
```

Out[319]=

```
1.
```

In[320]:=

```
Δ = {}; (* List of the norm of the differences *)
```

In[321]:=

```
ϵ = 10^-6;(* Convergence precision *)
G = B + ϵ;

While[Norm[B - G] > ϵ,
 AppendTo[Δ, Norm[B - G]];
 (* Append the norm of the difference to the Δ list *)
 B = G; (* Overwrite the previous eigenvalues *)
 F = H + Q.B.B; (* Calculate the matrix F each iteration *)
 {λ, ψ} = Eigensystem[{F, S}];
 {λ, ψ} = {λ[[#]], ψ[[#]]} &@Ordering[λ];
 (* Order the eigenvalues always in the same way for correctness *)
 G = MatrixNormalize[First@ψ, S];
 (* Normalize the minimal eigenvector w.r.t. the overlap matrix S *)
 If[G.S.G ≠ 1, Abort[], Nothing];(* Perform a numerical divergence check *)
]
```

In[324]:=

```
γ = Quantity[2 H.B.B + Q.B.B.B.B, "HartreeEnergy"]
(* Ground energy in Hartree energies *)
```

$$\text{Abs}\left[\frac{\gamma - -2.903\,E_h}{-2.903\,E_h}\right] \text{ // PercentForm}$$

Out[324]=

$-2.85516\,E_h$

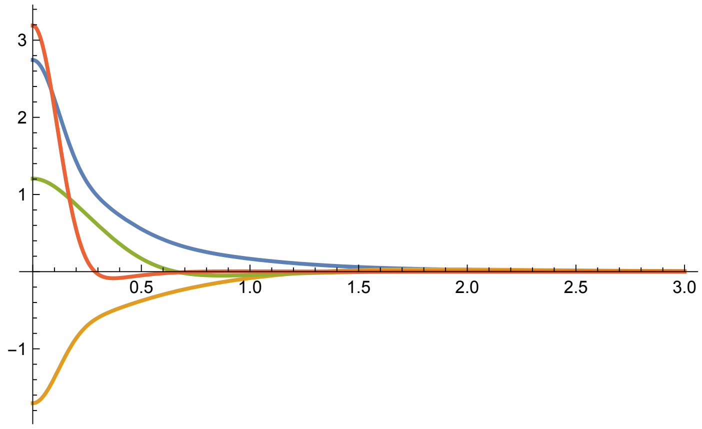
Out[325]//PercentForm=

```
1.648%
```

In[326]:=

```
Ψ = #.Array[χ[α#] &, {4}] & /@ψ;
Plot[Ψ, {r, 0, 3}, PlotRange → Full, PlotLegends → Placed["Expressions", Below]]
```

Out[327]=



$1.42119\, e^{-38.475 r^2} + 0.866291\, e^{-5.78295 r^2} + 0.384959\, e^{-1.24257 r^2} + 0.0707194\, e^{-0.298073 r^2}$

$-0.96176\, e^{-38.475 r^2} - 0.296127\, e^{-5.78295 r^2} - 0.54995\, e^{-1.24257 r^2} + 0.103159\, e^{-0.298073 r^2}$

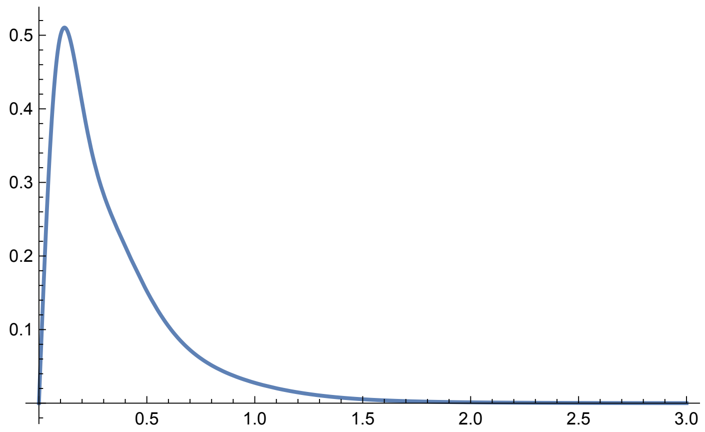
$0.104244\, e^{-38.475 r^2} + 1.28628\, e^{-5.78295 r^2} - 0.197489\, e^{-1.24257 r^2} + 0.0126622\, e^{-0.298073 r^2}$

$3.43228\, e^{-38.475 r^2} - 0.261344\, e^{-5.78295 r^2} + 0.0195436\, e^{-1.24257 r^2} - 0.00109799\, e^{-0.298073 r^2}$

In[328]:=

```
Plot[r Abs[First@Ψ]^2, {r, 0, 3}, PlotRange → Full]
```

Out[328]=



In[329]:=

```
ListStepPlot[Drop[Δ, 1], PlotRange → Full]
(* Measurements give 0.05 seconds for the convergence time for an SCF loop *)
```

Out[329]=