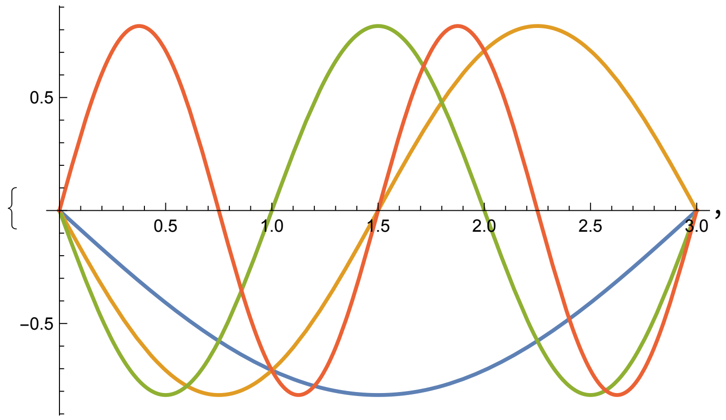
In[∘]:=
```
Charting`$InteractiveHighlighting = False
```
Out[∘]=
```
False
```

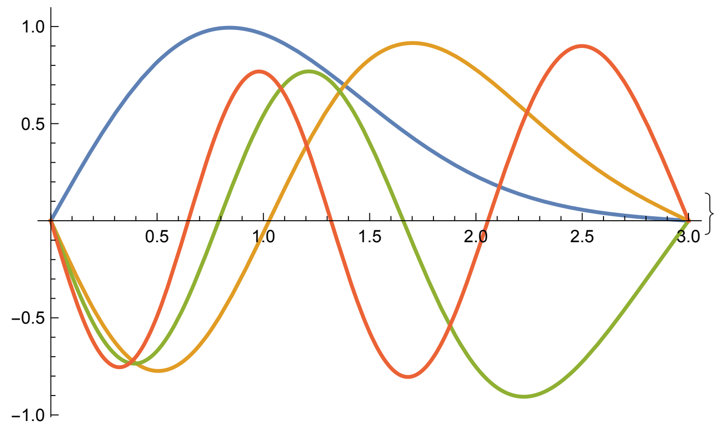
In[∘]:=
```
n = 9; (* Number of eigenstates *)
rMax = 3; (* Size of the box *)
int[r_] := {r, 0, rMax};
```

In[∘]:=
```
V[r_] := Piecewise[{{0, Abs[r] < rMax}, {∞, True}}];
```

In[∘]:=
```
{{efn1, evl1}, {efn2, evl2}} = NDEigensystem[{-1/2 Laplacian[u[r], {r}] + # u[r],
     DirichletCondition[u[r] == 0, True]}, u[r], int[r], n,
    Method → {"SpatialDiscretization" → {"FiniteElement", {"MeshOptions" →
          {"MaxCellMeasure" → 10^-3}}}}] & /@ {V[r], r^2} // Transpose;
```

In[∘]:=
```
Plot[Take[#, 4] // Evaluate, int[r], PlotRange → All, ImageSize → Medium] & /@
 {efn2, evl2}
```
Out[∘]=





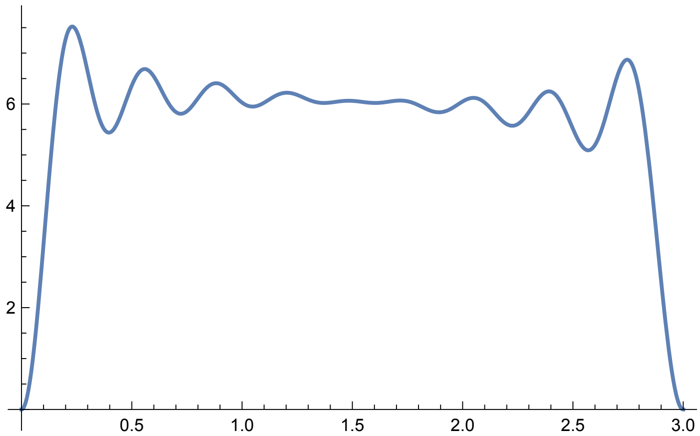
In[∘]:=
```
Sort[#] & /@ {efn1, evl1} // Column
```
Out[∘]=
```
{0.548311, 2.19325, 4.9348, 8.77298, 13.7078, 19.7392, 26.8673, 35.0919, 44.4132}
{2.12169, 4.97382, 8.07278, 11.918, 16.8133, 22.8152, 29.9239, 38.1356, 47.4478}
```

In[∘]:=
```
evalsSq = Abs[#]^2 & /@ evl2;
```

In[ ]:=
```
NIntegrate[#, int[r], PrecisionGoal → 4] & /@ evalsSq
```
Out[ ]=
```
{1., 1., 1., 1., 1., 1., 1., 1., 1.}
```

In[ ]:=
```
If[OddQ[n],
 list = 2 & /@ Range[1, n - 1];
 AppendTo[list, 1],
 list = 2 & /@ Range[1, n]
]
Length@list
```
Out[ ]=
```
{2, 2, 2, 2, 2, 2, 2, 2, 1}
```
Out[ ]=
```
9
```

In[ ]:=
```
rho[l_] := list.evalsSq /. {r → l};
Plot[rho[r], int[r], PlotRange → All]
```
Out[ ]=



In[ ]:= ldaEn = $-\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}$ NIntegrate[rho[r]$^{4/3}$, int[r], PrecisionGoal → 4]

Out[ ]=
```
-22.7635
```

In[ ]:= ldaPot = $-\left(\frac{3}{\pi}\right)^{1/3}$ rho[r]$^{1/3}$;

In[ ]:= enHart = $\frac{1}{2}$ NIntegrate[$\frac{\text{rho[r] rho[l]}}{\text{Abs[r - l]}^2}$, int[r], int[l], PrecisionGoal → 3]

NIntegrate : Numerical integration converging too slowly; suspect one of the following: singularity, value of the integration is 0, highly oscillatory integrand, or WorkingPrecision too small.

NIntegrate : NIntegrate failed to converge to prescribed accuracy after 18 recursive bisections in r near {r, l} = {1.5, 2.53237 }. NIntegrate obtained 7.706616315408025` *^8 and 1.1280364916524449` *^8 for the integral and error estimates.

Out[ ]=
3.85331×10^{8}

In[ ]:= potHart = Integrate[$\frac{\text{rho[l]}}{\sqrt{(\text{r - l})^2 + \epsilon}}$, int[r]];

In[ ]:=
```
(* Actual self-consistent loop for the Kohn-Sham equations *)
{evalKs, efnKs} =
  NDEigensystem[{-1/2 Laplacian[u[r], {r}] + (potHart[r] + ldaPot + r^2) u[r],
    DirichletCondition[u[r] == 0, True]},
   u[r], int[r], n, Method → {"SpatialDiscretization" →
     {"FiniteElement", {"MeshOptions" → {"MaxCellMeasure" → 10^-3}}}}];
```

NDEigensystem : The PDE coefficient

$$-r^2 + \left(\frac{3}{\pi}\right)^{1/3} \left(2\,\text{Abs}[\ll 21 \gg[\ll 5 \gg][\ll 1 \gg]]^2 + 2 \ll 1 \gg^2 + \ll 5 \gg + 2 \ll 1 \gg + \text{Abs}[\ll 1 \gg]^2\right)^{1/3} - \left(\int_0^3 \frac{1}{\sqrt{\text{Plus}[\ll 2 \gg]^2 + \epsilon}} \left(2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2 \ll 1 \gg^2 + 2 \ll 1 \gg^2 + 2 \ll 1 \gg^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + \text{Abs}[\text{InterpolatingFunction}[\ll 5 \gg][\ll 1 \gg]]^2\right) dr\right)[r]$$

does not evaluate to a numeric scalar at the coordinate {1.5}; it evaluated to

$$-0.454459 - \left(\int_0^3 \frac{1}{\sqrt{\text{Plus}[\ll 2 \gg]^2 + \epsilon}} \left(2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + \ll 4 \gg + 2\,\text{Abs}[\ll 1 \gg]^2 + \right.\right.$$

NDEigensystem : The PDE coefficient

$$-r^2 + \left(\frac{3}{\pi}\right)^{1/3} \left(2\,\text{Abs}[\ll 21 \gg[\ll 5 \gg][\ll 1 \gg]]^2 + 2 \ll 1 \gg^2 + \ll 5 \gg + 2 \ll 1 \gg + \text{Abs}[\ll 1 \gg]^2\right)^{1/3} - \left(\int_0^3 \frac{1}{\sqrt{\text{Plus}[\ll 2 \gg]^2 + \epsilon}} \left(2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2 \ll 1 \gg^2 + 2 \ll 1 \gg^2 + 2 \ll 1 \gg^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + \text{Abs}[\text{InterpolatingFunction}[\ll 5 \gg][\ll 1 \gg]]^2\right) dr\right)[r]$$

does not evaluate to a numeric scalar at the coordinate {1.5}; it evaluated to

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NDEigensystem : The PDE coefficient

$$-r^2 + \left(\frac{3}{\pi}\right)^{1/3} \left(2\,\text{Abs}[\ll 21 \gg[\ll 5 \gg][\ll 1 \gg]]^2 + 2 \ll 1 \gg^2 + \ll 5 \gg + 2 \ll 1 \gg + \text{Abs}[\ll 1 \gg]^2\right)^{1/3} - \left(\int_0^3 \frac{1}{\sqrt{\text{Plus}[\ll 2 \gg]^2 + \epsilon}} \left(2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2 \ll 1 \gg^2 + 2 \ll 1 \gg^2 + 2 \ll 1 \gg^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + \text{Abs}[\text{InterpolatingFunction}[\ll 5 \gg][\ll 1 \gg]]^2\right) dr\right)[r]$$

does not evaluate to a numeric scalar at the coordinate {1.5}; it evaluated to

$$-0.454459 - \left(\int_0^3 \frac{1}{\sqrt{\text{Plus}[\ll 2 \gg]^2 + \epsilon}} \left(2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + 2\,\text{Abs}[\ll 1 \gg]^2 + \ll 4 \gg + 2\,\text{Abs}[\ll 1 \gg]^2 + \right.\right.$$

General : Further output of NDEigensystem::femcnsd will be suppressed during this calculation.

Set : Lists {evalKs, efnKs } and

NDEigensystem $\left[\left\{u[r]\left(r^2 - \text{Times}[\ll 2 \gg]^{1/3}\ \text{Plus}[\ll 9 \gg]^{1/3} + \left(\int_0^3 \text{Power}[\ll 2 \gg]\ \text{Plus}[\ll 9 \gg]\, dr\right)[r]\right) - \frac{u''[r]}{2},\right.\right.$

DirichletCondition [u[r] == 0, True]}, u[r], {r, 0, 3 }, 9, Method → {SpatialDiscretization → {FiniteElement, {

MeshOptions → {≪1≫}}}}]

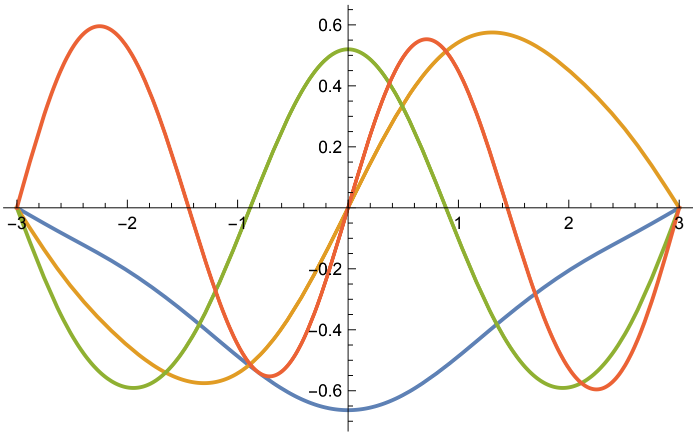
are not the same shape.

Out[ ]=

```
$Aborted
```

```
Plot[Take[efnKs, 4] // Evaluate, int[r], PlotRange → All]
```

Out[ ]=




```
Min[evalKs]
```

Out[ ]=

```
17.3663
```