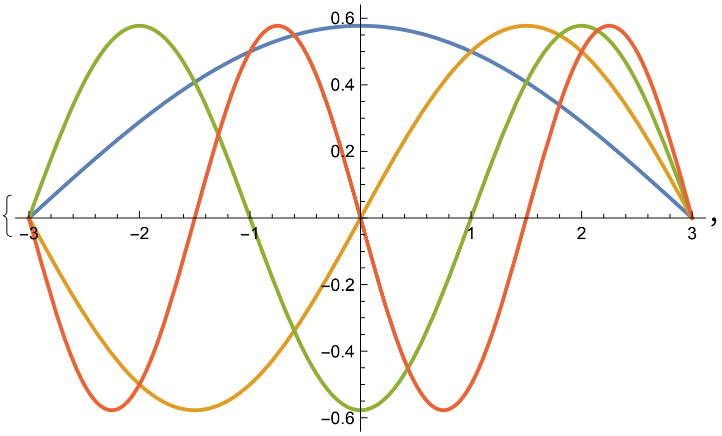
In[80]:=
```
n = 9; (* Number of eigenstates *)
L = 3; (* Size of the box *)
δ[x_] := {x, -L, L};
```

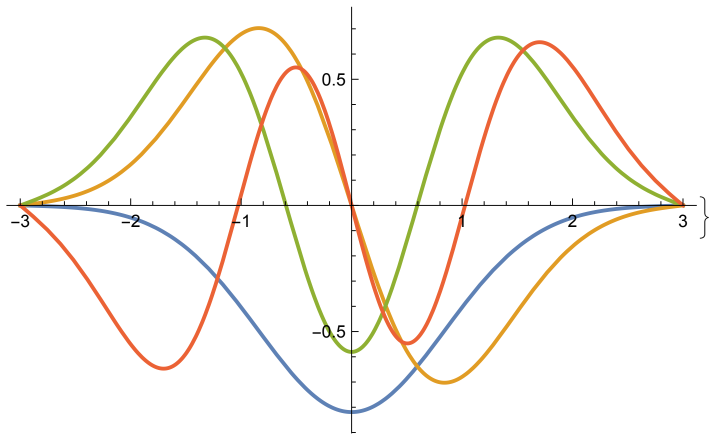
In[83]:=
```
V[x_] := Piecewise[{{0, Abs[x] < L}, {10^6, True}}];
```

In[84]:=
```
{{μ, λ}, {ϕ, ψ}} = NDEigensystem[{{-1/2 Laplacian[u[x], {x}] + # u[x],
      DirichletCondition[u[x] == 0, True]}, u[x], δ[x], n,
    Method → {"SpatialDiscretization" → {"FiniteElement", {"MeshOptions" →
          {"MaxCellMeasure" → 10^-3}}}}] & /@ {V[x], x^2} // Transpose;
```

In[85]:=
```
Plot[Take[#, 4] // Evaluate, δ[x], PlotRange → All, ImageSize → Medium] & /@ {ϕ, ψ}
```

Out[85]=





In[86]:=
```
Sort[#] & /@ {μ, λ} // Column
```

Out[86]=

```
{0.137078, 0.548311, 1.2337, 2.19325, 3.42695, 4.9348, 6.71681, 8.77298, 11.1033}
{0.707123, 2.12169, 3.53943, 4.97382, 6.46302, 8.07278, 9.87433, 11.918, 14.2281}
```

In[87]:=
```
β = Abs[#]^2 & /@ ψ;
```

In[88]:=
```
NIntegrate[#, δ[x], PrecisionGoal → 4] & /@ β
```

Out[88]=

```
{1., 1., 1., 1., 1., 1., 1., 1., 1.}
```

In[89]:=
```
If[OddQ[n],
 ν = 2 & /@ Range[1, n - 1];
 AppendTo[ν, 1],
 ν = 2 & /@ Range[1, n]
]
Length@ν
```

Out[89]=

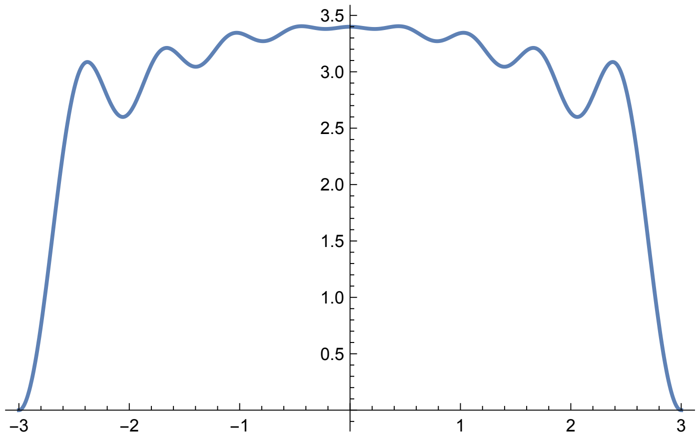
{2, 2, 2, 2, 2, 2, 2, 2, 1}

Out[90]=

9

In[91]:=
```
ρ[y_] := ν.β /. {x → y};
Plot[ρ[x], δ[x], PlotRange → All]
```

Out[92]=



In[93]:= $E_{LDA} = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}$ NIntegrate$\left[\rho[x]^{4/3}, \delta[x], \text{PrecisionGoal} \to 4\right]$

Out[93]=

-18.213

In[94]:= $v_{LDA} = -\left(\frac{3}{\pi}\right)^{1/3} \rho[x]^{1/3};$

In[95]:= $\epsilon = 10^{-2}$ // N;

$E_{Ha} = \frac{1}{2}$ NIntegrate$\left[\frac{\rho[x] \times \rho[y]}{\sqrt{(x-y)^2+\epsilon}}, \delta[x], \delta[y], \text{PrecisionGoal} \to 3\right]$

Out[96]=

198.876

In[97]:= Δ = N@Subdivide$\left[-L, L, 10^2\right]$;

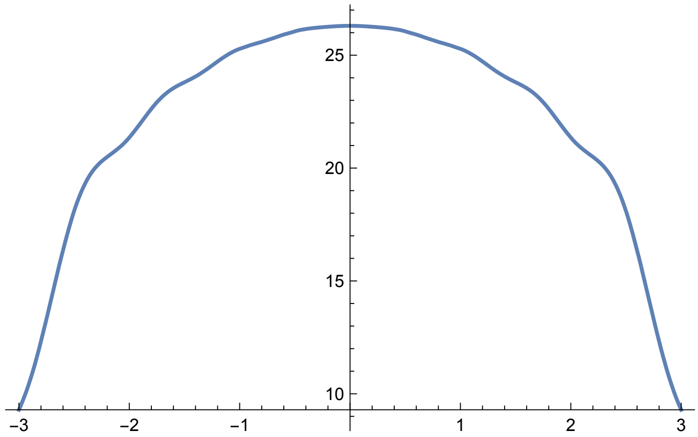
$v_{Ha,values}$ = NIntegrate$\left[\frac{\rho[y]}{\sqrt{(\#-y)^2+\epsilon}}, \delta[y], \text{PrecisionGoal} \to 3\right]$ & /@ Δ;

In[99]:= v_{Ha} = Interpolation[Transpose[{Δ, $v_{Ha,values}$}], InterpolationOrder → 5];

In[100]:=

```
Plot[vHa[x], δ[x]]
```

Out[100]=



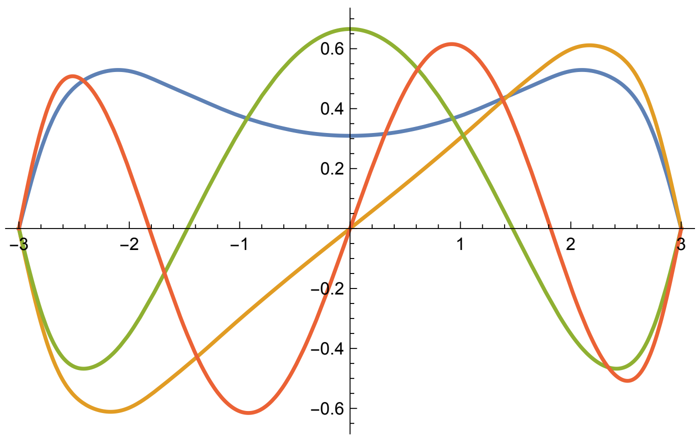
In[101]:=

```
(* Actual self-consistent loop for the Kohn-Sham equations *)
{ℰ, υ} = NDEigensystem[{-1/2 Laplacian[u[x], {x}] + (vHa[x] + vLDA + x^2) u[x],
    DirichletCondition[u[x] == 0, True]},
   u[x], δ[x], n, Method → {"SpatialDiscretization" →
      {"FiniteElement", {"MeshOptions" → {"MaxCellMeasure" → 10^-3}}}}];
```

In[102]:=

```
Plot[Take[υ, 4] // Evaluate, δ[x], PlotRange → All]
```

Out[102]=



In[103]:=

```
Min[ℰ]
```

Out[103]=

```
24.6116
```