Chem 540_2018
A Quick Look @ Mathematica !

Function_Name[Variables_] // Define a function

In[1]:=

In[23]:=
```
blue[x_, a_] := (x^2) * Exp[-a * x^2]
```

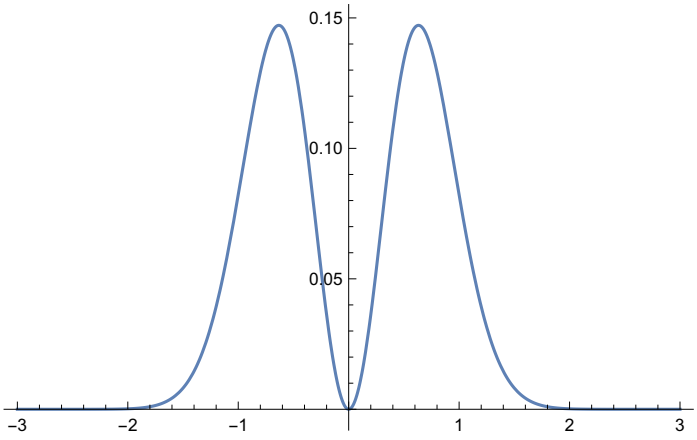
```
Exp[x^2]
```

Out[24]= e^{x^2}

Plotting Functions
Plot[Function_Name[Variables],{Ind. Variable, Lower Lim, Upper Lim}]

```
Plot[blue[x, 2.5], {x, -3, 3}]
```

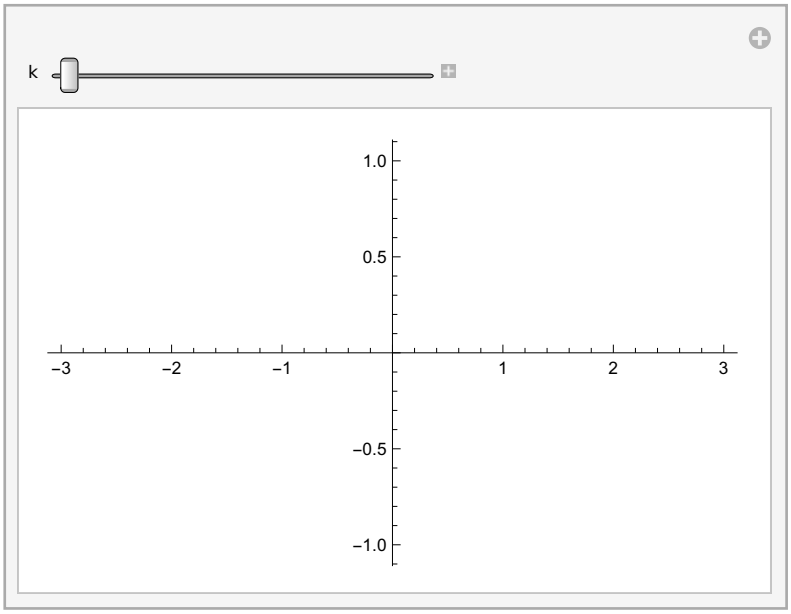
Out[25]=



Manipulate a function

```
Manipulate[Plot[{blue[x, k]}, {x, -3, 3}], {k, 0.1, 3}]
```

Out[26]=



Time for Calculus !!

In[27]:=
```
Clear[AInt]
```

```
AInt[k_] =
 Integrate[blue[x, k], {x, -Infinity, Infinity}, Assumptions → k > 0]
```

Out[28]= $\frac{\sqrt{\pi}}{2\,k^{3/2}}$

```
N[AInt[2.5]]
```

Out[29]= 0.2242

```
NIntegrate[blue[y, 2.5], {y, -5.0, 5.0}]
```

Out[30]= 0.2242

In[31]:=

```
D[blue[x, k], {x, 0}]
```

Out[32]= $e^{-k\,x^2}\,x^2$

What's that function?

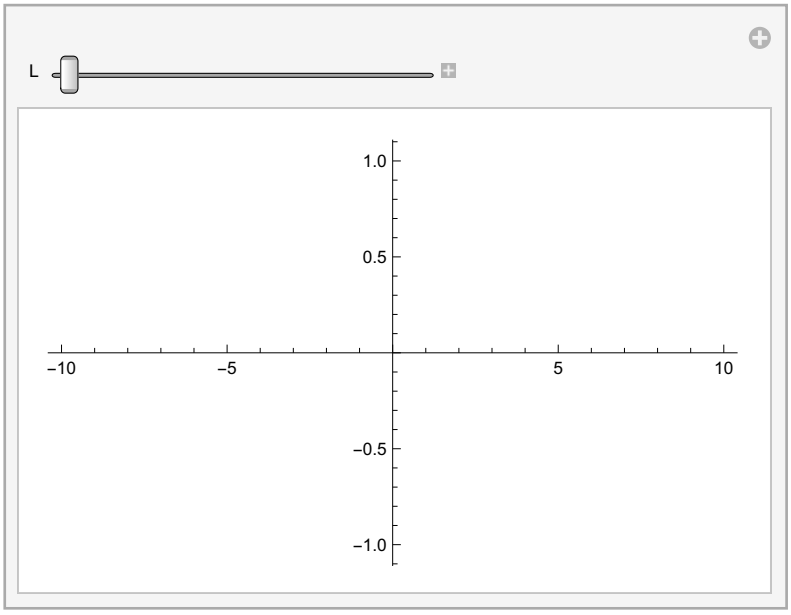
```
green[n_, L_, x_] = Sqrt[2 / L] * Sin[n * Pi * (x + L / 2) / L]
```

Out[33]= $\sqrt{2}\,\sqrt{\frac{1}{L}}\,\text{Sin}\left[\frac{n\,\pi\,\left(\frac{L}{2}+x\right)}{L}\right]$

In[34]:=

```
Manipulate[Plot[{green[2, L, x]}, {x, -10, 10}], {L, 0.5, 3}]
```

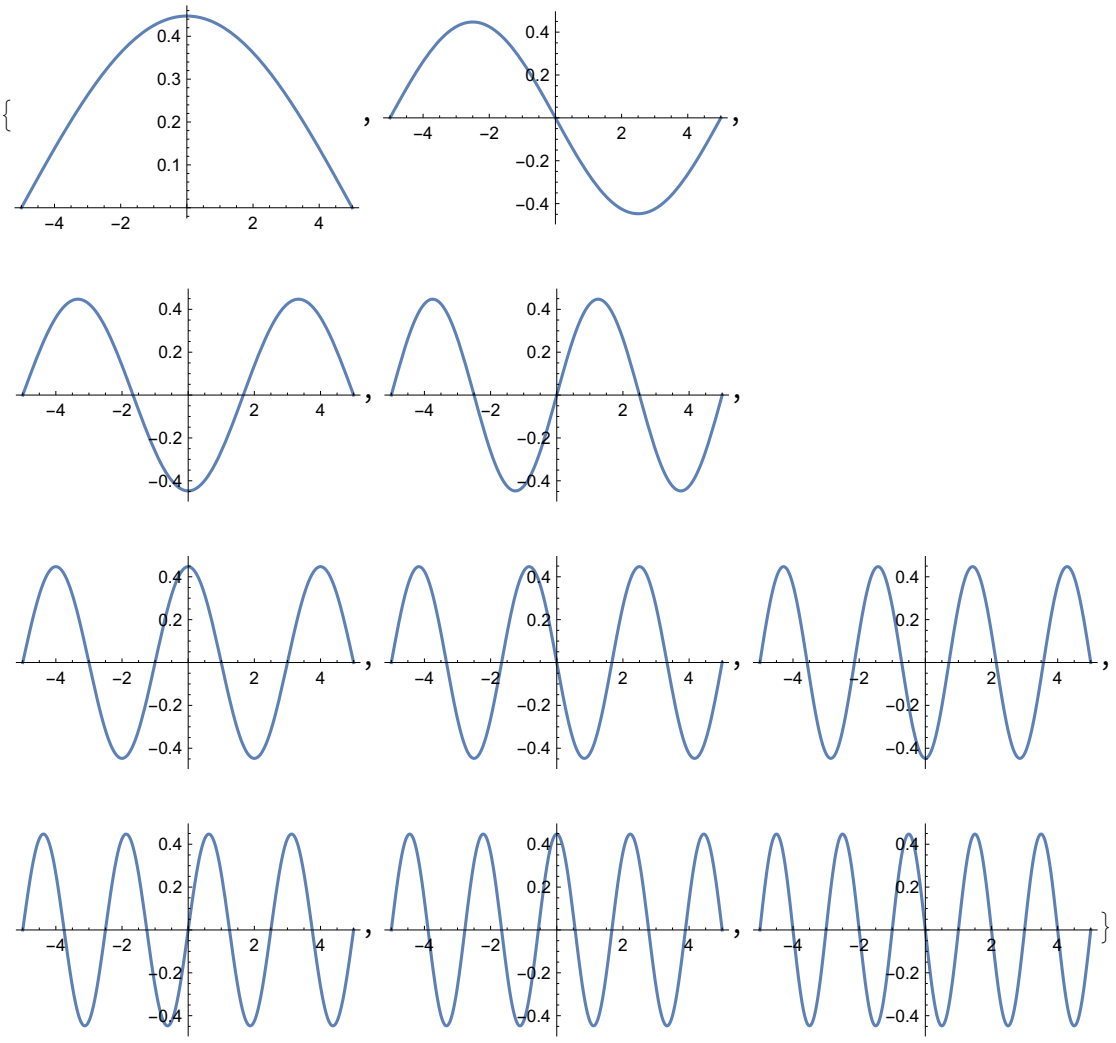
Out[35]=



When you have to repeat operations

```
Table[Plot[green[n, 10, x], {x, -5, 5}], {n, 1, 10}]
```

Out[36]=



In[37]:=

In[38]:=

Matrices

```
H = {{0, 1, 0}, {0, 2, 0}, {1, 1, 1}}
```

Out[39]= {{0, 1, 0}, {0, 2, 0}, {1, 1, 1}}

```
EVal = Eigenvalues[H]
```

Out[40]= {2, 1, 0}

```
Evec = Eigenvectors[H]
```

Out[41]= {{1, 2, 3}, {0, 0, 1}, {-1, 0, 1}}

In[42]:=

In[43]:=

In[44]:=