In[47]:=
```
<< VariationalMethods`
```

Introducing Lagrange's equation:

In[48]:=
```
(*Introducing Kinetic energy 'T' and potential energy 'U' for N atoms*)
T[t_, N_] := 1/2 (Sum[x_l'[t]^2, {l, 1, N}])
U[t_, N_] := 1/2 ω_0^2 (x_1[t]^2 + x_N[t]^2 + Sum[(x_i[t] - x_(i-1)[t])^2, {i, 2, N}])
```

In[50]:=
```
(* Defining the Lagrangian to be L = T - U*)
L[N_] := T[t, N] - U[t, N]
```

In[51]:=
```
(* Using mathematica to apply Euler's
 equation on 'L' to find the equations of motion*)
EoM[N_, j_] := EulerEquations[L[N], Subscript[x, j][t], t]
```

In[52]:=
```
(* Showing the equation of motion for the first,
middle, and the last atom for a system of 3 atoms*)
```

In[53]:=
```
Expand@EoM[3, 1] // TraditionalForm (* the equation of motion of the first atom*)
```

Out[53]//TraditionalForm=

$$-x_1''(t) - 2\,x_1(t) + x_2(t) = 0$$

In[54]:=
```
Expand@EoM[3, 2] // TraditionalForm(* the equation of motion of the middle atom*)
```

Out[54]//TraditionalForm=

$$-x_2''(t) + x_1(t) - 2\,x_2(t) + x_3(t) = 0$$

In[55]:=
```
Expand@EoM[3, 3] // TraditionalForm(* the equation of motion of a final atom*)
```

Out[55]//TraditionalForm=

$$-x_3''(t) + x_2(t) - 2\,x_3(t) = 0$$

Constructing the matrix D_n and evaluating its eigenmodes:

In[56]:=
```
(* Intorducing Dn, the matrix of the coefficients of the equations of motion*)
Dn[N_] := Table[Coefficient[-ω0^2 (x_(i-1)[t] - 2 x_i[t] + x_(i+1)[t]), x_j[t]], {i, N}, {j, N}];

(* Introducing Dω which simply a diagonal matrix with ω^2 in its diagonal *)
Dω[N_] := DiagonalMatrix[Table[ω^2, {i, N}], 0, N];

(*Evaluatong Dn[5] and Dn[5]-Dω[5] to show a sample of the matrix we will solve*)
MatrixForm@Dn[5] // TraditionalForm
MatrixForm@(Dn[5] - Dω[5]) // TraditionalForm
```

Out[58]//TraditionalForm=

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{pmatrix}$$

Out[59]//TraditionalForm=

$$\begin{pmatrix} 2-\omega^2 & -1 & 0 & 0 & 0 \\ -1 & 2-\omega^2 & -1 & 0 & 0 \\ 0 & -1 & 2-\omega^2 & -1 & 0 \\ 0 & 0 & -1 & 2-\omega^2 & -1 \\ 0 & 0 & 0 & -1 & 2-\omega^2 \end{pmatrix}$$

In[60]:=
```
(* Setting ω0 = 1 for numerical Computation *)
ω0 = 1;
```

In[61]:=
```
(*Defining the Eigenmodes of Dn*)
EigValSol[n_] := Eigenvalues[N[Dn[n]]];
```

In[62]:=
```
(* Solving the eigenvalues for N = 1700 atom, then save it in a variable *)
ListOfSol = EigValSol[1700];
```

Defining the density of state and plot it alongside the plot of eigenmodes' distribution:

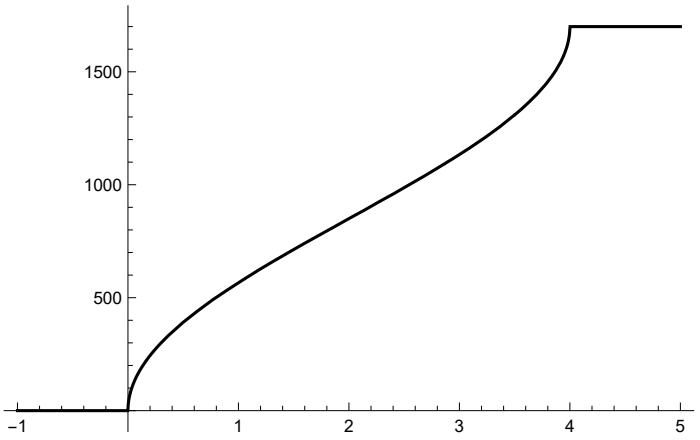
In[63]:=
```
(* The length of 'Cases' function will
 return the number of eigenmodes that are less than ω*)
NLω[ω_] := Length@Cases[ListOfSol, λ_ /; λ < ω]
```

In[64]:=
```
(* Defining the density of state and taking dω=0.01 for smooth curve,
less than this value will cause fluctuations due to the numerical approach *)
ρ[ω_, dω_] := (NLω[ω + dω] - NLω[ω])/dω
```

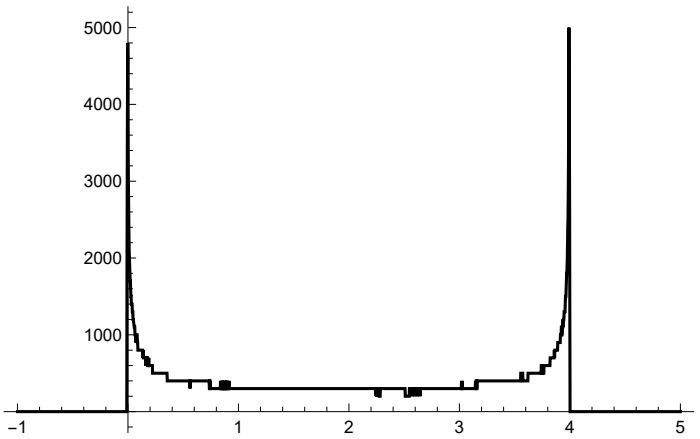
In[65]:=
```
(* Plotting the Number of Eigenmodes that is
 less than ω and its derivative: The density of state*)
```

In[66]:=
```
Plot[NLω[ω], {ω, -1, 4 ω0^2 + 1}, PlotPoints → 45,
 MaxRecursion → 6, PlotRange → All, PlotStyle → Black]
Plot[ρ[ω, 0.01], {ω, -1, 4 ω0^2 + 1}, PlotPoints → 45,
 MaxRecursion → 6, PlotRange → All, PlotStyle → Black]
```

Out[66]=

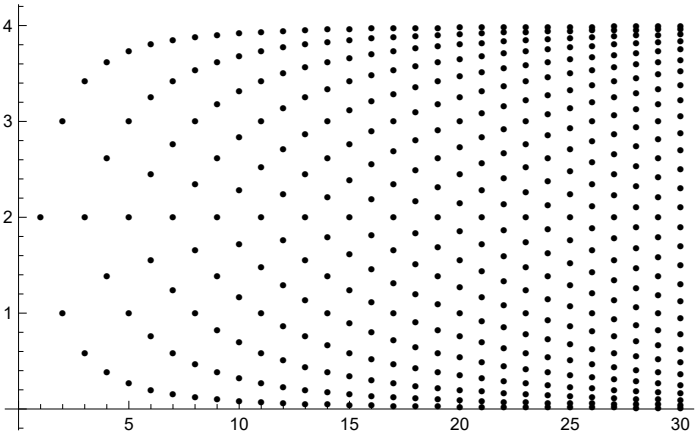


Out[67]=



In[68]:=
```
(* The distribution of the Eigenmodes of the matrix Dn *)
Show[Table[DiscretePlot[EigValSol[l], {n, l, l}, Filling → None, PlotStyle → {Black},
   PlotMarkers → {"•", Medium}], {l, 30}], PlotRange → {{0, 30}, {0, 4}}]
```

Out[68]=

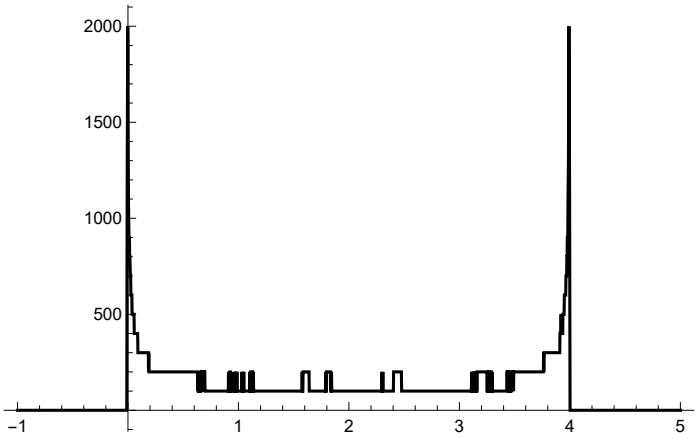


Investigation the relationship between ω^2_0 and ω^2_{max} .

Define ω^2_{max} to be the value of ω that the density of state will converge to zero afterwards , for lets take $\omega^2_0 = 1$, lets observe the value of ω^2_{max}

In[69]:=
```
ω₀ = 1;
ListOfSol = EigValSol[700];
Plot[ρ[ω, 0.01], {ω, -1, 5}, PlotPoints → 45,
 MaxRecursion → 6, PlotRange → All, PlotStyle → Black]
```

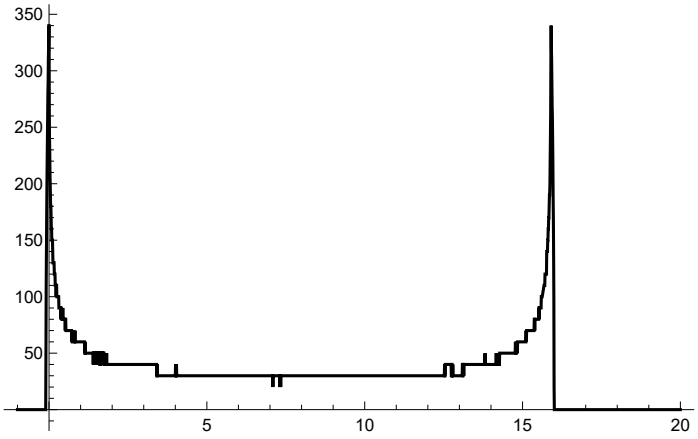
Out[71]=



The value of ω^2_{max} for $\omega_0 = 1$ was $\omega^2_{max} = 4$, Now we will take $\omega_0 = 2 \rightarrow \omega^2_0 = 4$, and we will observe ω^2_{max}

In[72]:=
```
ω₀ = 2;
ListOfSol = EigValSol[700];
Plot[ρ[ω, 0.1], {ω, -1, 20}, PlotPoints → 45,
 MaxRecursion → 6, PlotRange → All, PlotStyle → Black]
```

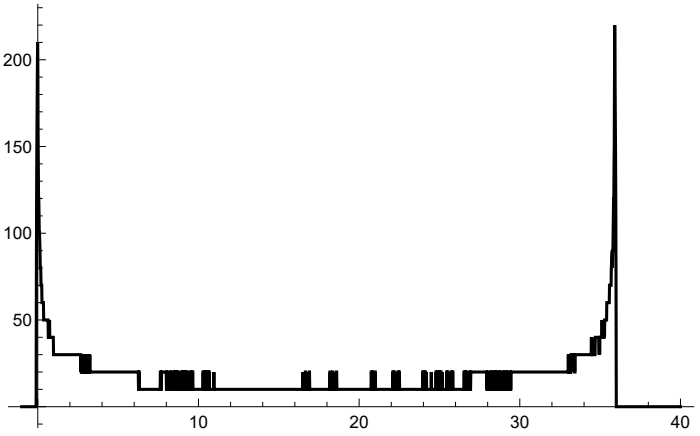
Out[74]=



The value of ω^2_{max} for $\omega_0 = 2$ was $\omega^2_{max} = 16$, Now we will take $\omega_0 = 3 \rightarrow \omega^2_0 = 9$, and we will observe ω^2_{max}

In[75]:=
```
ω0 = 3;
ListOfSol = EigValSol[700];
Plot[ρ[ω, 0.1], {ω, -1, 40}, PlotPoints → 45,
 MaxRecursion → 6, PlotRange → All, PlotStyle → Black]
```

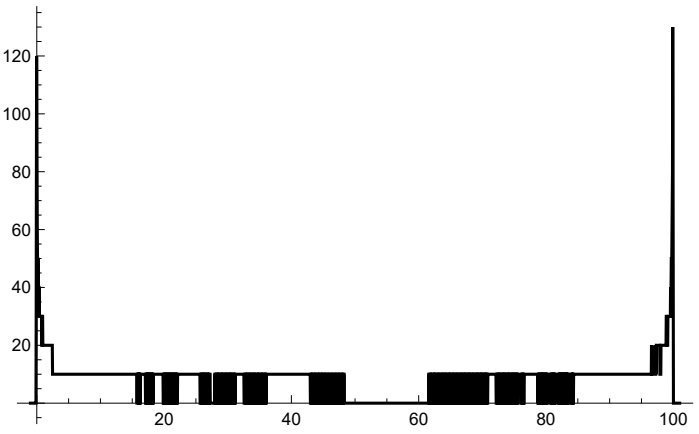
Out[77]=



The value of ω^2_{max} for $\omega_0 = 3$ was $\omega^2_{max} = 36$, We can now describe the relationship between ω^2_{max} and ω^2_0 by this empirical formula: $\omega^2_{max} = 4\,\omega^2_0$, we can verify it by choosing a value of ω^2_0 then predict the value of ω^2_{max} and check if we were accurate. Lets take $\omega_0 = 5 \rightarrow \omega^2_0 = 25$, we predict ω^2_{max} to be 100:

In[78]:=
```
ω0 = 5;
ListOfSol = EigValSol[700];
Plot[ρ[ω, 0.1], {ω, -1, 4 ω0^2 + 1}, PlotPoints → 45,
 MaxRecursion → 6, PlotRange → All, PlotStyle → Black]
```

Out[80]=



The empirical formula $\omega^2_{max} = 4\,\omega^2_0$ appears to work fine for this system of atoms.