In[61]:=
```
(*
 MATHEMATICA DEMO OF METROPOLIS MONTE CARLO
  METHOD FOR PARTICLES ON A SQUARE LATTICE
  WITH NEAREST–NEIGHBOR INTERACTIONS
 *)
<< Graphics`MultipleListPlot`
 $TextStyle = {FontSize → 16}
(*
 INITIALIZE LATTICE DIMENSIONS
  AND MAXIMUM NUMBER OF MCS
 *)
L = 8;
LTOT = L^2;
HalfL = L / 2;
NA = LTOT / 2;
NB = LTOT - NA;
MCS = 1000;
MaxTrials = MCS LTOT + 1;
(*
 INITIALIZE INTERACTIONS AND UNIT VECTORS
 *)
ϵAA = 0.0;
ϵBB = 0.0;
ϵAB = -1.0;
uvex = {0, 1, 0, -1};
uvey = {1, 0, -1, 0};
(*
 INITIALIZE THE LATTICE
 *)
Np = 0;
lattice = Table[0, {i, L}, {j, L}];
Alist = Table[0, {i, NA}, {j, 2}];
Blist = Table[0, {i, NB}, {j, 2}];
TotE = Table[0, {i, 1, MaxTrials}];
Do[{Np = Np + 1;
   lattice[[i, j]] = 1;
   Alist[[Np, 1]] = i;
   Alist[[Np, 2]] = j}, {i, 1, L}, {j, 1, HalfL}];
Np = 0;
Do[{Np = Np + 1;
   lattice[[i, j]] = 2;
   Blist[[Np, 1]] = i;
   Blist[[Np, 2]] = j}, {i, 1, L}, {j, HalfL + 1, L}];
(*
 OBTAIN THE INITIAL TOTAL ENERGY
```

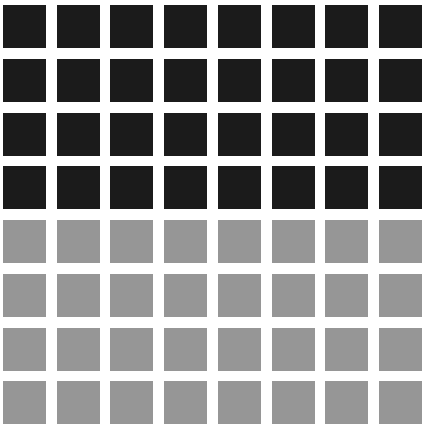
```
 *)
TotE[[1]] = 0;
Do[{
  (*
   First, Get the Neighbors
   *)
  xNN = i + uvex[[k]];
  (*
   Periodic Boundary Conditions
   *)
  If[xNN > L, xNN = 1];
  If[xNN < 1, xNN = L];
  yNN = j + uvey[[k]];
  If[yNN > L, yNN = 1];
  If[yNN < 1, yNN = L];
  (*
   Obtain Energy
   *)
  If[lattice[[i, j]] == 1,
   {If[lattice[[xNN, yNN]] == 1,
     TotE[[1]] = TotE[[1]] + ϵAA,
     TotE[[1]] = TotE[[1]] + ϵAB]},
   {If[lattice[[xNN, yNN]] == 1,
     TotE[[1]] = TotE[[1]] + ϵAB,
     TotE[[1]] = TotE[[1]] + ϵBB]}]}, {i, 1, L}, {j, 1, L}, {k, 1, 4}];
TotE[[1]] = TotE[[1]] / 2.0 ;
Print["Initial Lattice Configuration"];
MultipleListPlot[{Alist, Blist}, Axes → False,
  AspectRatio → Automatic, PlotRange → {{-2, L + 2}, {-2, L + 2}}, SymbolShape →
   {PlotSymbol[Box, 10.0, Filled → True], PlotSymbol[Box, 10.0, Filled → True]},
  SymbolStyle → {RGBColor[0, 1, 0], RGBColor[0, 0, 1]}];
(*
 THE MONTE CARLO LOOP
 *)
Do[{
   (*
    First, Select an A and B at Random
    *)
   SiteA = Random[Integer, {1, NA}];
   SiteB = Random[Integer, {1, NB}];
   (*
    Get the Coordinates of the A and B sites
    *)
   xa = Alist[[SiteA, 1]];
   ya = Alist[[SiteA, 2]];
   xb = Blist[[SiteB, 1]];
```

```
yb = Blist[[SiteB, 2]];
(*
 Get the Neighbors and Calculate the Energies
 *)
Aold = 0;
Bold = 0;
Anew = 0;
Bnew = 0;
Do[{
  (*
   First, Get the Neighbors of A
   *)
  xNNA = xa + uvex[[i]];
  (*
   Periodic Boundary Conditions
   *)
  If[xNNA > L, xNNA = 1];
  If[xNNA < 1, xNNA = L];
  yNNA = ya + uvey[[i]];
  If[yNNA > L, yNNA = 1];
  If[yNNA < 1, yNNA = L];
  (*
   Obtain Energies Before and After Exchange with B
   *)
  If[xNNA == xb && yNNA == yb,
   {Aold = Aold + ϵAB; Bnew = Bnew + ϵAB},
   {If[lattice[[xNNA, yNNA]] == 1,
     {Aold = Aold + ϵAA; Bnew = Bnew + ϵAB},
     {Aold = Aold + ϵAB; Bnew = Bnew + ϵBB}]}];
  (*
   Get the Neighbors of B
   *)
  xNNB = xb + uvex[[i]];
  If[xNNB > L, xNNB = 1];
  If[xNNB < 1, xNNB = L];
  yNNB = yb + uvey[[i]];
  If[yNNB > L, yNNB = 1];
  If[yNNB < 1, yNNB = L];
  (*
   Obtain Energies Before and After Exchange with A
   *)
  If[xNNB == xa && yNNB == ya,
   {Bold = Bold + ϵAB; Anew = Anew + ϵAB},
   {If[lattice[[xNNB, yNNB]] == 1,
     {Bold = Bold + ϵAB; Anew = Anew + ϵAA},
     {Bold = Bold + ϵBB; Anew = Anew + ϵAB}]}]}, {i, 1, 4}];
```

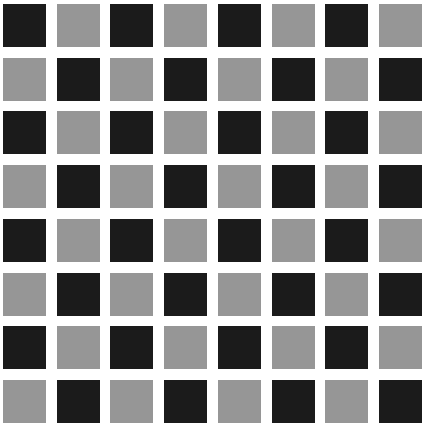
```
(*
 Obtain Initial and Final Energies
  and Move with Metropolis Probabilities
 *)
Told = Aold + Bold;
Tnew = Anew + Bnew;
If[Tnew ≤ Told,
 {Alist[[SiteA, 1]] = xb;
  Alist[[SiteA, 2]] = yb;
  Blist[[SiteB, 1]] = xa;
  Blist[[SiteB, 2]] = ya;
  lattice[[xa, ya]] = 2;
  lattice[[xb, yb]] = 1;
  TotE[[trials]] = TotE[[trials - 1]] - Told + Tnew},
 {boltz = Exp[-(Tnew - Told)];
  p = Random[];
  If[p < boltz,
   {Alist[[SiteA, 1]] = xb;
    Alist[[SiteA, 2]] = yb;
    Blist[[SiteB, 1]] = xa;
    Blist[[SiteB, 2]] = ya;
    lattice[[xa, ya]] = 2;
    lattice[[xb, yb]] = 1;
    TotE[[trials]] = TotE[[trials - 1]] - Told + Tnew},
   {TotE[[trials]] = TotE[[trials - 1]]};]}], {trials, 2, MaxTrials}];
TotE = TotE / LTOT;
Print["Final Lattice Configuration"];
MultipleListPlot[{Alist, Blist}, Axes → False,
  AspectRatio → Automatic, PlotRange → {{-2, L + 2}, {-2, L + 2}}, SymbolShape →
   {PlotSymbol[Box, 10.0, Filled → True], PlotSymbol[Box, 10.0, Filled → True]},
  SymbolStyle → {RGBColor[0, 1, 0], RGBColor[0, 0, 1]}];
ListPlot[TotE, PlotJoined → True, PlotRange → All, AxesOrigin → 0,
  Frame → True, FrameLabel → {"Trials", "Energy"}];
```

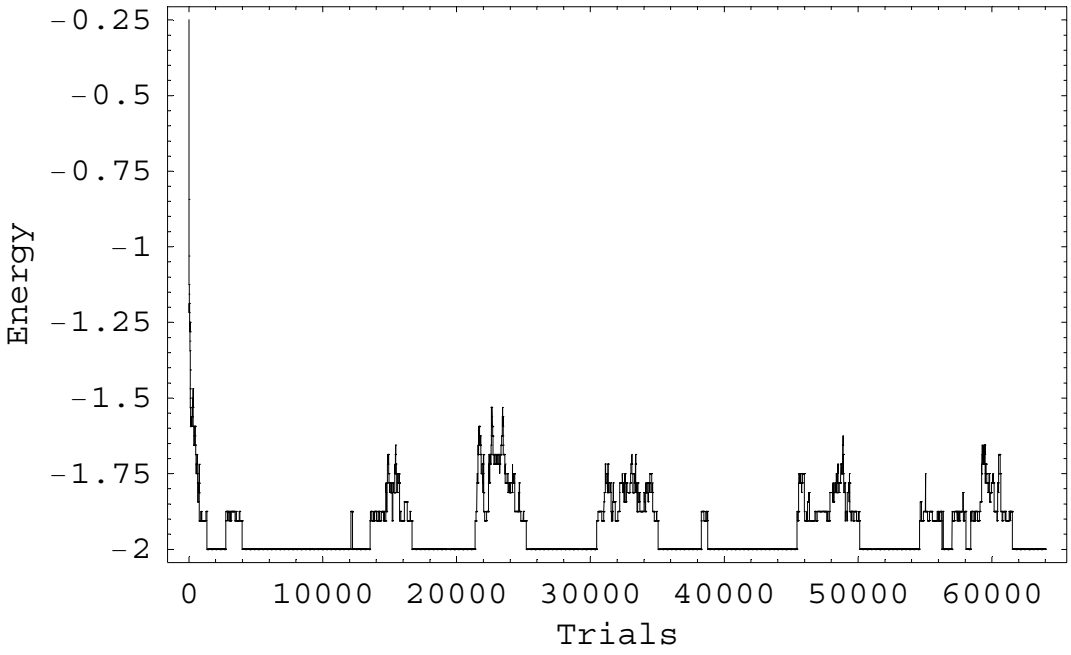
Out[61]= {Null (FontSize → 16)}

Initial Lattice Configuration



Final Lattice Configuration




-0.25
-0.5
-0.75
-1
-1.25
-1.5
-1.75
-2
Energy
0
10000
20000
30000
40000
50000
60000
Trials