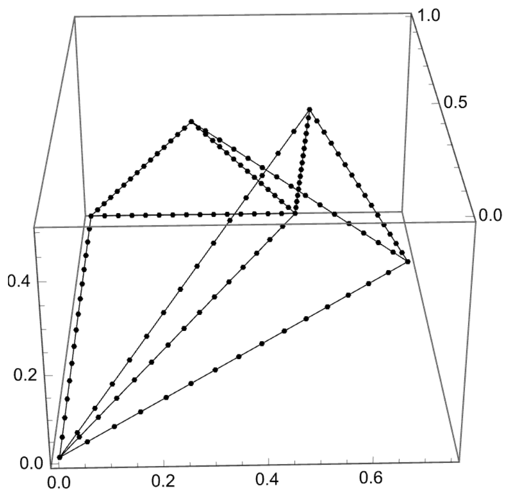
In[84]:=
```
Charting`$InteractiveHighlighting = False
```
Out[84]=
```
False
```
In[85]:=
```
SetOptions[SelectedNotebook[],
 PrintingStyleEnvironment → "Printout", ShowSyntaxStyles → True]
```
In[86]:=
```
n = 15; (* Points to sample along each connection *)
```
In[87]:=
```
path = N@With[{Γ = {0, 0, 0}, X = {0, 1, 0}, W = {1/2, 1, 0}, L = {1/2, 1/2, 1/2},
     K = {3/4, 3/4, 0}, U = {1/4, 1, 1/4}}, {L, K, U, W, Γ, X, W, L, Γ, K, U, X}];
(* The list of high-symmetry points *)
kPts = N@Subdivide[#1, #2, n] & @@@ Partition[path, 2, 1] // Flatten[#, 1] & //
   DeleteAdjacentDuplicates; (* List of n points sampled along
  each line of the path going through the high-symmetry points,
it's literally the points generated by traversing the line,
although not in equal steps *)
Length@kPts (* Total count of the sampling points *)
Graphics3D[{Point[#] & /@ kPts, Line[path]}, Axes → True]
```
Out[89]=
```
166
```
Out[90]=

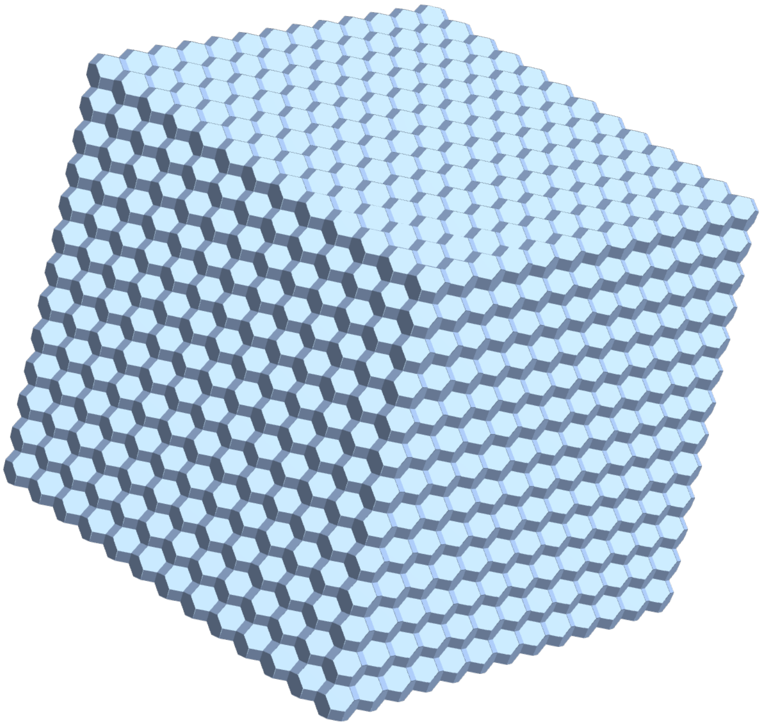


In[91]:=
```
basis = N@{{1, -1, 1}, {1, 1, -1}, {-1, 1, 1}}; (* The basis for the G *)
G = Tuples[N@Range[-7, 7], 3].basis;
(* All possible combinations that give the G points *)
Length@G (* Number of sampled points *)
(* 1BZ represented for a bcc lattice *)
eee = VoronoiMesh[G];
hm = HighlightMesh[eee, Style[2, Directive[Red]]];
eee = MeshRegion[MeshCoordinates[hm], MeshCells[hm, {3, "Interior"}]]
```

Out[93]=

```
3375
```

Out[96]=



In[97]:=

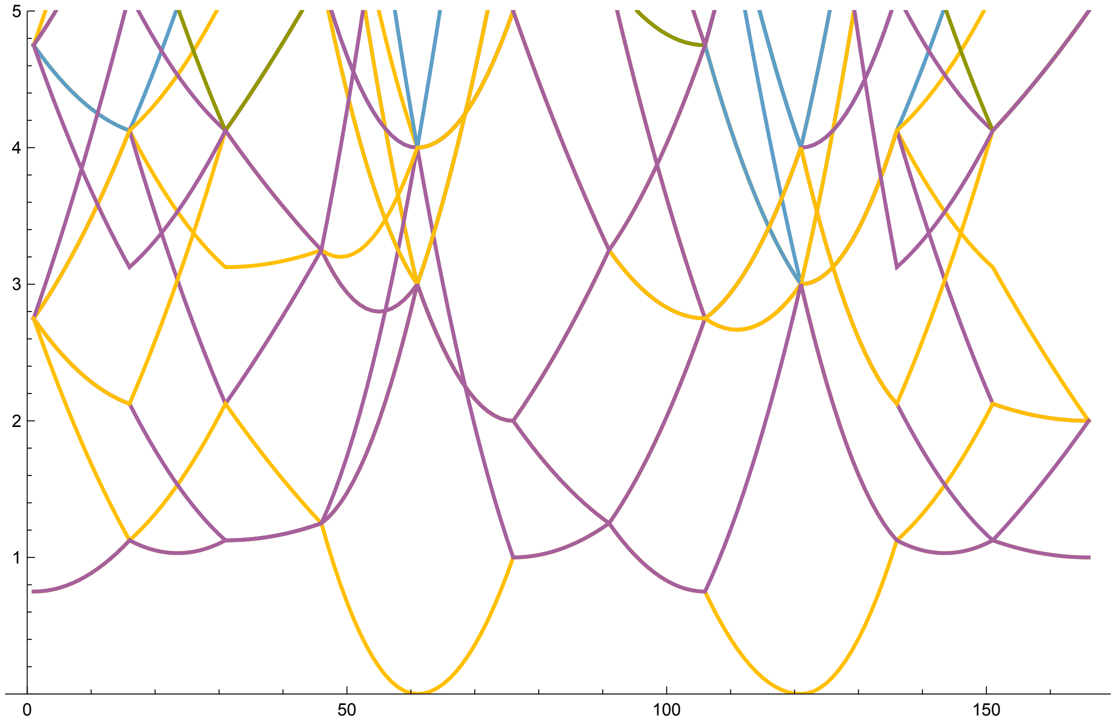
In[98]:=
```
(*Export["~/Downloads/test3d.stl",
 MeshPrimitives[BoundaryMesh[eee],2]//RegionUnion,"STL"]*)
```

In[99]:=

In[100]:=

```
ens = With [{allCombs = Tuples[{kPts, G}] // Partition[#, Length@G] &},
    Norm[#1 - #2]^2 & @@@ # & /@ allCombs] // Transpose;
(* Energy levels calculated along the path traced in the
 first Brillouin zone for a bcc lattice *)
ListLinePlot[ens, ImageSize → Large, PlotRange → {0, 5}]
```

Out[101]=



3D DOS (bulk)

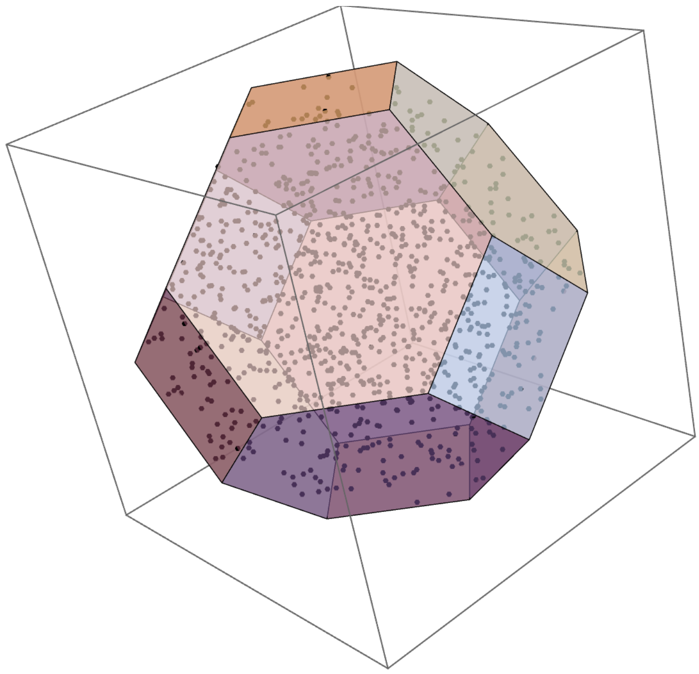
In[102]:=

```
firstBz = With[{G = Tuples[Range[-1, 1], 3].basis}, Select[
    MeshPrimitives[VoronoiMesh[G], 3], RegionMember[#, {0, 0, 0}] &] // First];
```

In[103]:=

```
kPts = RandomPoint[firstBz, 10^3];
Graphics3D[{Style[firstBz, Opacity[0.7]], Point@kPts}]
RegionMeasure[firstBz]
```

Out[104]=



Out[105]=

```
4.
```

In[106]:=

```
(*Export["~/Downloads/firstBz.stl",firstBz,"STL"]*)
```

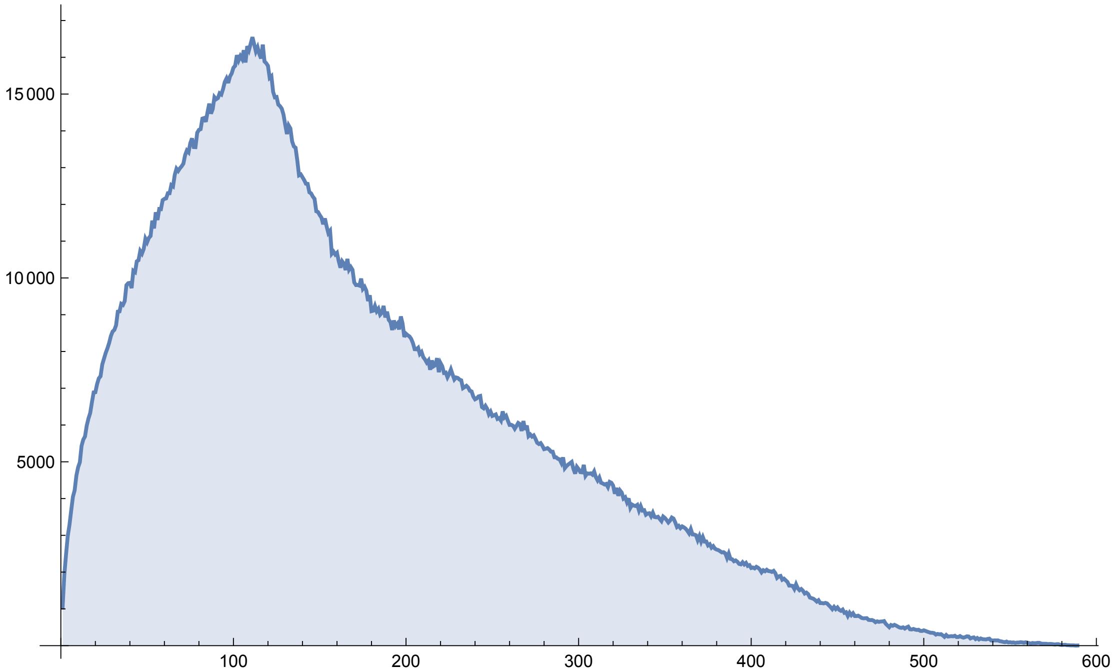
In[107]:=

```
G = Tuples[N@Range[-7, 7], 3].basis;
(* All possible combinations that give the G points *)
allCombs = Tuples[{kPts, G}] // Partition[#, Length@G] &;
eVals = Norm[#1 - #2]^2 & @@@ # & /@ allCombs // Transpose;
```

In[110]:=

```
(* Plot of the density of states as a function of energy *)
Show[BinCounts[Flatten@eVals] //
   ListLinePlot[#, ImageSize → Large, Filling → Axis, PlotRange → All] &,
 Plot[dosFit["BestFit"], {x, 0, 130}, PlotStyle → {Dashed, Orange, Thick}],
 PlotRange → All]
```

Out[110]=

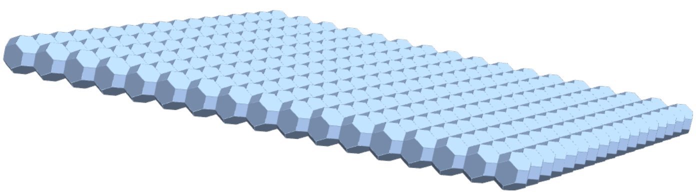


2D DOS part (quantum well)

In[111]:=

```
n = 1;
basis2d = {{1, -1, 1}, {1, 1, -1}, {-1, 1, 1}}; (* The basis for the G *)
gen = Select[Tuples[Range[-9, 9], 3], Abs[#[[3]]] ≤ n &];
G2d = gen.basis2d;
vm = VoronoiMesh[G2d];
hm = HighlightMesh[vm, Style[2, Directive[Red]]];
vm = MeshRegion[MeshCoordinates[hm], MeshCells[hm, {3, "Interior"}]]
```

Out[117]=



In[118]:=

```
(*Export["~/Downloads/test2d.stl",
 MeshPrimitives[BoundaryMesh[vm],2]//RegionUnion,"STL"]*)
```

In[119]:=

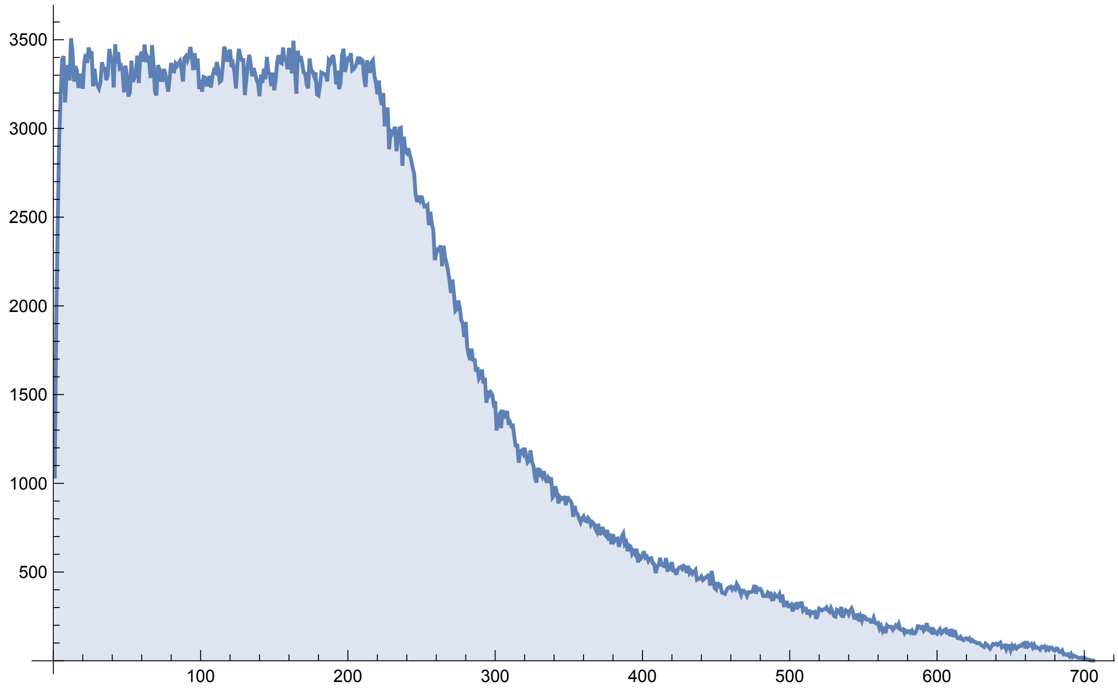
In[120]:=

```
allCombs = Tuples[{kPts, G2d}] // Partition[#, Length@G2d] &;
eVals = Norm[#1 - #2]^2 & @@@ # & /@ allCombs // Transpose;
```

In[122]:=

```
(* Plot of the density of states as a function of energy *)
BinCounts[Flatten@eVals] //
 ListLinePlot[#, ImageSize → Large, PlotRange → All, Filling → Axis] &
```

Out[122]=



1D DOS part (quantum wire)

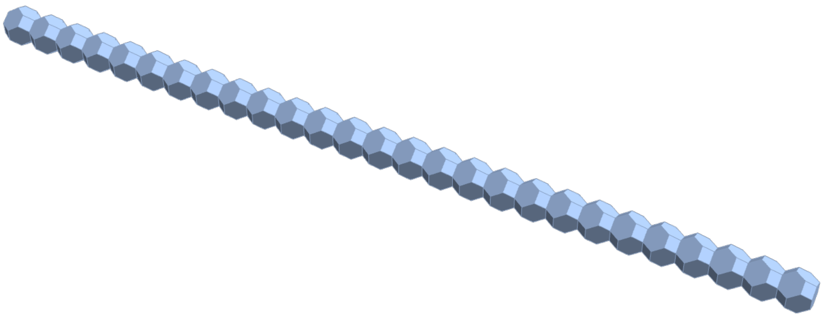
In[123]:=

```
n = 1
basis1d = {{1, -1, 1}, {1, 1, -1}, {-1, 1, 1}}; (* The basis for the G *)
gen1 =
  Select[Tuples[Range[-14, 14], 3], #[[3]] ≤ n && #[[3]] ≥ -n && #[[2]] ≤ n && #[[2]] ≥ -n &];
G1d = gen1.basis1d;
vm1 = VoronoiMesh[G1d];
hm = HighlightMesh[vm1, Style[2, Directive[Red]]];
vm1 = MeshRegion[MeshCoordinates[hm], MeshCells[hm, {3, "Interior"}]]
```

Out[123]=

1

Out[129]=



In[130]:=

```
mp = MeshPrimitives[BoundaryMesh[vm1], 2] // RegionUnion;
```

In[131]:=

```
(*Export["~/Downloads/test1d.stl",mp, "STL"]*)
```

In[132]:=

```
(*Export[
 "/Users/giovannigravili/Library/Mobile Documents/com~apple~CloudDocs/LM
   MANO/Computational material physics /Report for
   the exam/1dlattPlt.pdf",vm1,ImageResolution→800]*)
```

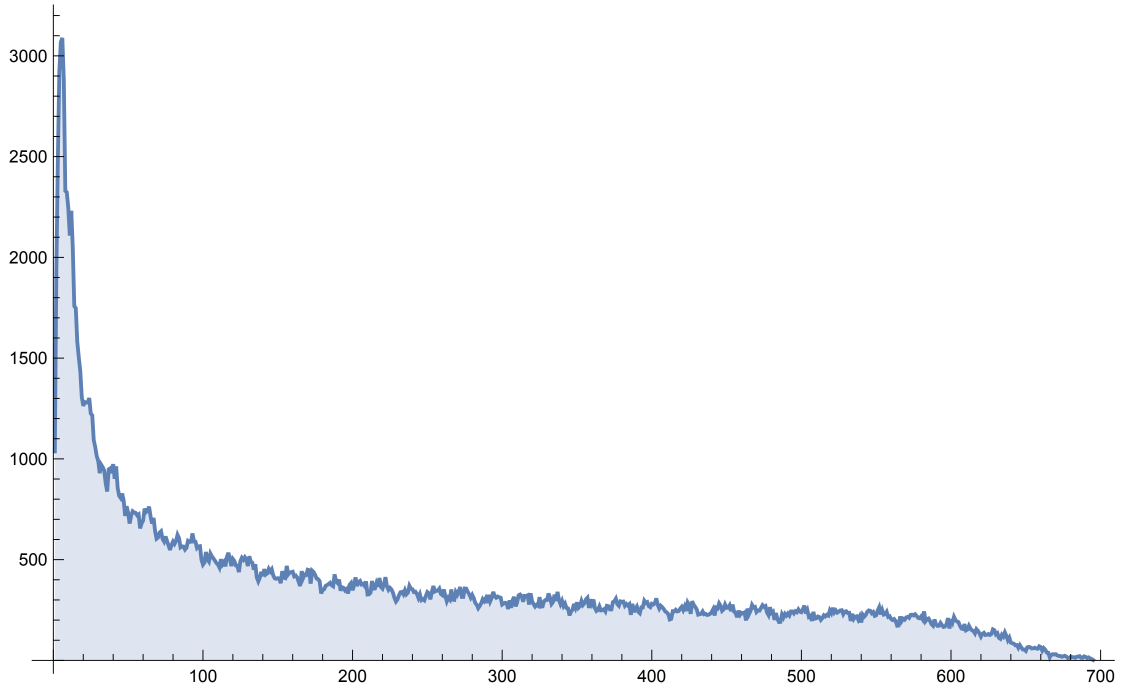
In[133]:=

```
allCombs = Tuples[{kPts, G1d}] // Partition[#, Length@G1d] &;
eVals = Norm[#1 - #2]^2 & @@@ # & /@ allCombs // Transpose;
```

In[135]:=

```
(* Plot of the density of states as a function of energy *)
BinCounts[Flatten@eVals] //
 ListLinePlot[#, ImageSize → Large, PlotRange → All, Filling → Axis] &
```

Out[135]=



0D DOS part (quantum dots)

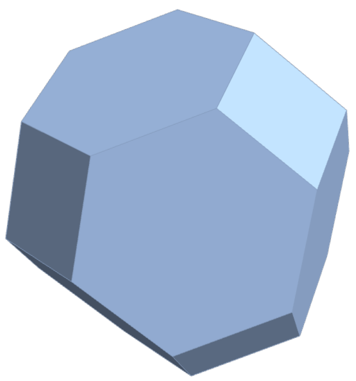
In[136]:=

```
n = 1
basis1d = {{1, -1, 1}, {1, 1, -1}, {-1, 1, 1}}; (* The basis for the G *)
gen1 = Select[Tuples[Range[-3, 3], 3],
   Abs[#[[3]]] ≤ n && Abs[#[[2]]] ≤ n && Abs[#[[1]]] ≤ n &];
G1d = gen1.basis1d;
vm1 = VoronoiMesh[G1d];
hm = HighlightMesh[vm1, Style[2, Directive[Red]]];
vm1 = MeshRegion[MeshCoordinates[hm], MeshCells[hm, {3, "Interior"}]]
```

Out[136]=

```
1
```

Out[142]=



In[143]:=

```
(*Printout3D[vm1]["FileName"][[1]]//CopyToClipboard*)
```

In[144]:=

```
allCombs = Tuples[{kPts, G1d}] // Partition[#, Length@G1d] &;
eVals = Norm[#1 - #2]^2 & @@@ # & /@ allCombs // Transpose;
```

In[146]:=

```
(* Plot of the density of states as a function of energy *)
BinCounts[Flatten@eVals] //
 ListPlot[#, ImageSize → Large, PlotRange → All, Filling → Axis] &
```

Out[146]=