

```
In[*]:= << Notation`
```

```
In[*]:= Notation[ $\left[ x_{[n\_]} \Leftrightarrow x_{n\_} \right]$ ]
```

```
In[*]:= (* All the numerical coefficients are defined at the beginning *)
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```
a = 1.;
```

```
m = 1.;
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```
 $\hbar$  = 0.1;
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```
In[*]:= n = 20;
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```
 $\xi$  = Range[ $-\frac{\pi}{2a}, \frac{\pi}{2a}, n$ ];
```

```
(* The interval of n k-values sampled along the interval *)
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```
In[*]:= 2 t Cos[]
```

```
*** Cos: Cos called with 0 arguments; 1 argument is expected.
```

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Out[*]=
```

```
2 t Cos[]
```

```
In[*]:= Array[ $\frac{\hbar \text{Norm}[\#]^2}{2m} + \# \delta \&, \{$ 
```

```
 $\beta = \text{N@}\{a \left\{ \frac{\sqrt{3}}{2}, \frac{1}{2} \right\}, a \left\{ \frac{\sqrt{3}}{2}, -\frac{1}{2} \right\}\};$ 
```

```
G = Tuples[Range[-2, 2], 2]. $\beta$ ;
```

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Length@G (* Number of sampled points *)
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(* 1BZ represented for a honeycomb lattice *)
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```
Show[VoronoiMesh[G, PlotTheme -> "Lines",
```

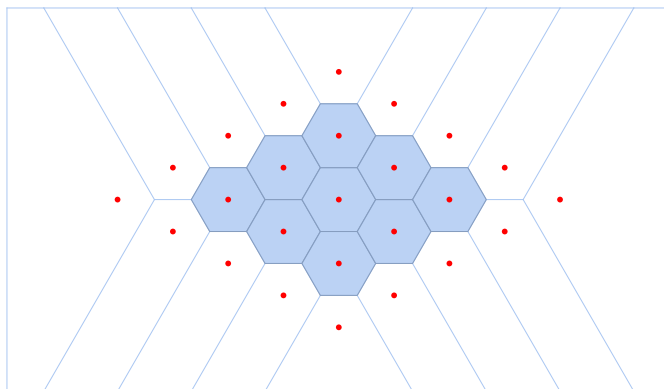
```
MeshCellStyle -> {{2, "Interior"} -> Directive[Opacity[0.8]]}],
```

```
Graphics[{Red, Point[G]}], PlotRange -> Automatic]
```

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Out[*]=
```

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25
```

```
Out[*]=
```



```

bas = N@{ $\frac{2\pi}{a\sqrt{3}}$  {1,  $\sqrt{3}$ },  $\frac{2\pi}{a\sqrt{3}}$  {1,  $-\sqrt{3}$ }};

path = N@With[{ $\Gamma = \{0, 0\}$ ,  $K = \{\frac{2}{3}, \frac{1}{3}\} \cdot \text{bas}$ ,  $M = \{\frac{1}{2}, \frac{1}{2}\} \cdot \text{bas}$ }, {M,  $\Gamma$ , K, M}];

(* The list of high-symmetry points *)
samplPts = 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@samplPts (* Total count of the sampling points *)
K = Tuples[Range[-1, 1], 2].bas;
Length@K (* Number of sampled points *)
Show[VoronoiMesh[K, PlotTheme -> "Lines",
MeshCellStyle -> {{2, "Interior"} -> Directive[Opacity[0.8]]}],
Graphics[{{Red, Point[K]}, {Thick, Line[path]}}],
PlotRange -> Automatic, Axes -> True]
Graphics[{Point[#] & /@ samplPts, Line[path]}, Axes -> True]

```

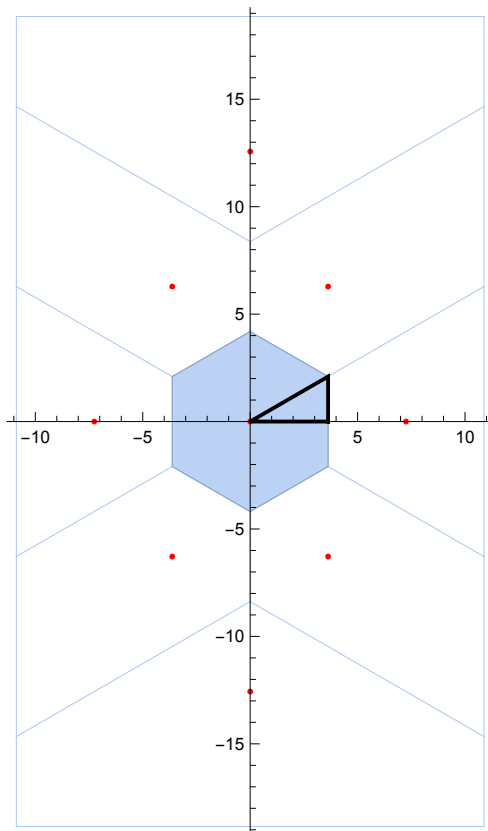
Out[*]=

61

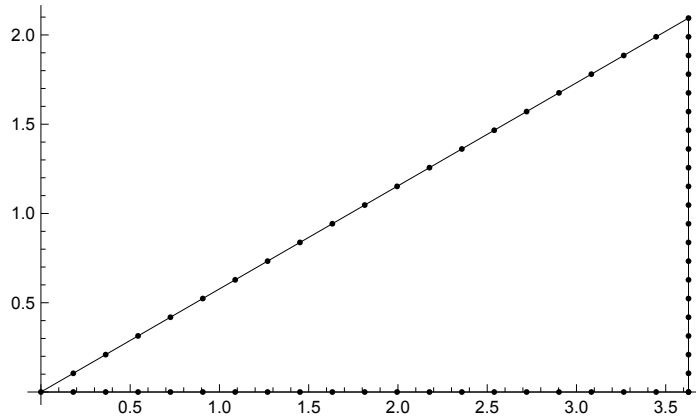
Out[*]=

9

Out[*]=



Out[*]=



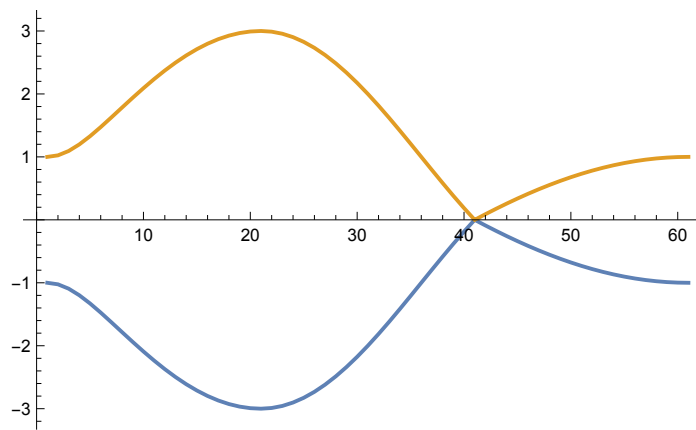
t = 1.;

fnband = t $\sqrt{3 + 2 \cos[a \#2] + 4 \cos\left[\frac{\sqrt{3}}{2} a \#1\right] \cos\left[\frac{a}{2} \#2\right]}$ &@@@ samplPts;

pm[a_] := {-a, a};

ListLinePlot[± fnband, PlotRange → Automatic]

Out[*]=



In[*]:=