In[1]:=
```
a1 = a * {Sqrt[3] / 2, 1 / 2}
```

Out[1]=
$$\left\{\frac{\sqrt{3}\ a}{2}, \frac{a}{2}\right\}$$

In[2]:=
```
a2 = a * {-Sqrt[3] / 2, 1 / 2}
```

Out[2]=
$$\left\{-\frac{\sqrt{3}\ a}{2}, \frac{a}{2}\right\}$$

In[3]:=
```
a3 = a * {0, -1}
```

Out[3]=
$$\{0, -a\}$$

In[7]:=
```
b1 = -a2;
b2 = -a3; b3 = -a1;
```

In[9]:=
```
k = {kx, ky}
```

Out[9]=
$$\{kx, ky\}$$

In[10]:=
```
k * a1
```

Out[10]=
$$\left\{\frac{1}{2}\sqrt{3}\ a\ kx, \frac{a\ ky}{2}\right\}$$

In[14]:=
```
Dot[k, a1]
```

Out[14]=
$$\frac{1}{2}\sqrt{3}\ a\ kx + \frac{a\ ky}{2}$$

In[25]:=
```
A = {{ϵ0 - ϵ, -t * (Exp[I * Dot[k, a1]] + Exp[I * Dot[k, a2]] + Exp[I * Dot[k, a3]])},
  {-t * (Exp[I * Dot[k, b1]] + Exp[I * Dot[k, b2]] + Exp[I * Dot[k, b3]]), ϵ0 - ϵ}}
```

Out[25]=
$$\left\{\left\{-\epsilon + \epsilon 0, -\left(e^{-i\ a\ ky} + e^{i\left(-\frac{1}{2}\sqrt{3}\ a\ kx + \frac{a\ ky}{2}\right)} + e^{i\left(\frac{1}{2}\sqrt{3}\ a\ kx + \frac{a\ ky}{2}\right)}\right) t\right\},\right.$$
$$\left.\left\{-\left(e^{i\ a\ ky} + e^{i\left(-\frac{1}{2}\sqrt{3}\ a\ kx - \frac{a\ ky}{2}\right)} + e^{i\left(\frac{1}{2}\sqrt{3}\ a\ kx - \frac{a\ ky}{2}\right)}\right) t, -\epsilon + \epsilon 0\right\}\right\}$$

In[26]:=
```
MatrixForm[A]
```

Out[26]//MatrixForm=
$$\begin{pmatrix} -\epsilon + \epsilon 0 & -\left(e^{-i\ a\ ky} + e^{i\left(-\frac{1}{2}\sqrt{3}\ a\ kx + \frac{a\ ky}{2}\right)} + e^{i\left(\frac{1}{2}\sqrt{3}\ a\ kx + \frac{a\ ky}{2}\right)}\right) t \\ -\left(e^{i\ a\ ky} + e^{i\left(-\frac{1}{2}\sqrt{3}\ a\ kx - \frac{a\ ky}{2}\right)} + e^{i\left(\frac{1}{2}\sqrt{3}\ a\ kx - \frac{a\ ky}{2}\right)}\right) t & -\epsilon + \epsilon 0 \end{pmatrix}$$

In[28]:=
```
Solve[FullSimplify[Det[A], Element[{a, kx, ky}, Reals]] == 0, ϵ]
```

Out[28]=
$$\left\{\left\{\epsilon \to \epsilon 0 - \sqrt{3\,t^2 + 2\,t^2\,\text{Cos}\left[\sqrt{3}\,a\,kx\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx - 3\,ky\right)\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx + 3\,ky\right)\right]}\right\},\right.$$
$$\left.\left\{\epsilon \to \epsilon 0 + \sqrt{3\,t^2 + 2\,t^2\,\text{Cos}\left[\sqrt{3}\,a\,kx\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx - 3\,ky\right)\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx + 3\,ky\right)\right]}\right\}\right\}$$

In[29]:=
```
ϵ1 = ϵ0 - Sqrt[3 t^2 + 2 t^2 Cos[Sqrt[3] a kx] + 2 t^2 Cos[1/2 a (Sqrt[3] kx - 3 ky)] + 2 t^2 Cos[1/2 a (Sqrt[3] kx + 3 ky)]]
```

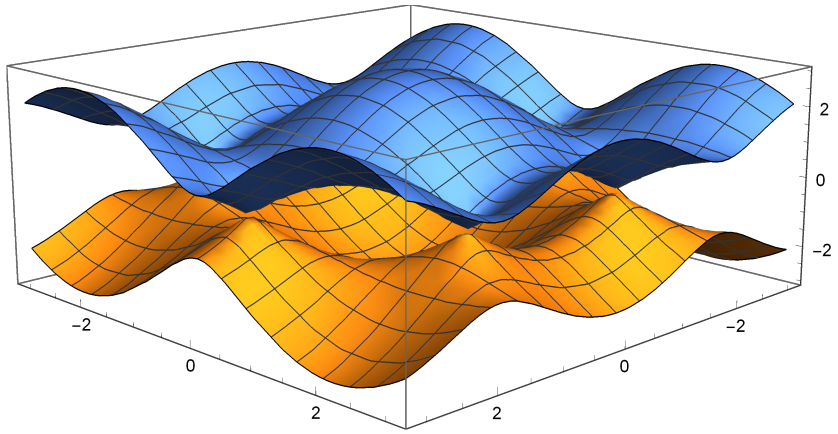
Out[29]=
$$\epsilon 0 - \sqrt{3\,t^2 + 2\,t^2\,\text{Cos}\left[\sqrt{3}\,a\,kx\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx - 3\,ky\right)\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx + 3\,ky\right)\right]}$$

In[30]:=
```
ϵ2 = ϵ0 + Sqrt[3 t^2 + 2 t^2 Cos[Sqrt[3] a kx] + 2 t^2 Cos[1/2 a (Sqrt[3] kx - 3 ky)] + 2 t^2 Cos[1/2 a (Sqrt[3] kx + 3 ky)]]
```

Out[30]=
$$\epsilon 0 + \sqrt{3\,t^2 + 2\,t^2\,\text{Cos}\left[\sqrt{3}\,a\,kx\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx - 3\,ky\right)\right] + 2\,t^2\,\text{Cos}\left[\frac{1}{2}\,a\left(\sqrt{3}\,kx + 3\,ky\right)\right]}$$

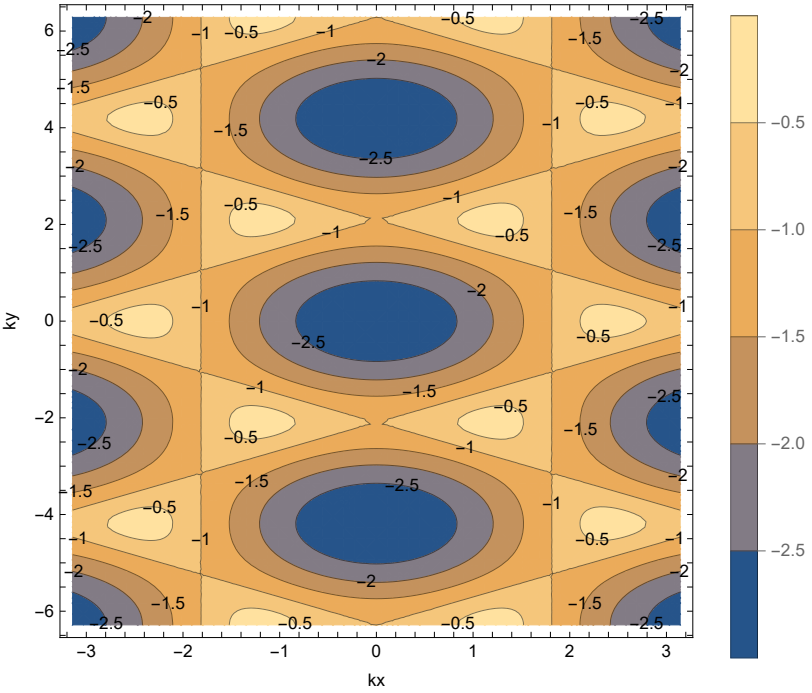
In[38]:=
```
Plot3D[{(ϵ1 - ϵ0) /. {t → 1, a → 1}, (ϵ2 - ϵ0) /. {t → 1, a → 1}}, {kx, -Pi, Pi}, {ky, -Pi, Pi}]
```

Out[38]=



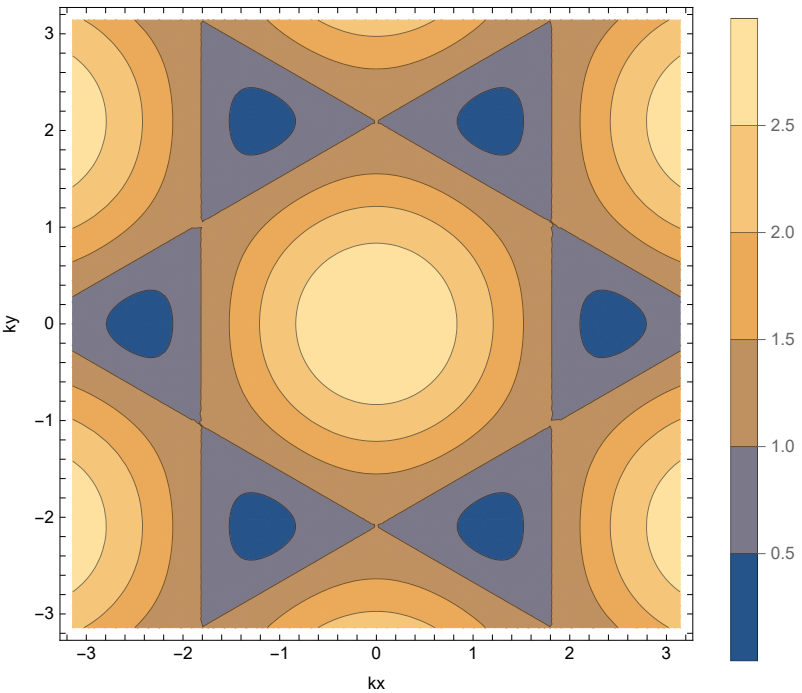
In[69]:=
```
ContourPlot[{(ϵ1 - ϵ0) /. {t → 1, a → 1}}, {kx, -Pi, Pi}, {ky, -2 * Pi, 2 * Pi},
 PlotLegends → Automatic, FrameLabel → {"kx", "ky"}, ContourLabels → True]
```

Out[69]=



In[57]:=
```
ContourPlot[{(ϵ2 - ϵ0) /. {t → 1, a → 1}}, {kx, -Pi, Pi},
 {ky, -Pi, Pi}, PlotLegends → Automatic, FrameLabel → {"kx", "ky"}]
```

Out[57]=



In[43]:=
```
FullSimplify[
  3 t^2 + 2 t^2 Cos[Sqrt[3] a kx] + 2 t^2 Cos[1/2 a (Sqrt[3] kx - 3 ky)] + 2 t^2 Cos[1/2 a (Sqrt[3] kx + 3 ky)]]
```

Out[43]= $t^2 \left(3 + 2 \cos\left[\sqrt{3}\, a\, kx\right] + 2 \cos\left[\frac{1}{2} a \left(\sqrt{3}\, kx - 3\, ky\right)\right] + 2 \cos\left[\frac{1}{2} a \left(\sqrt{3}\, kx + 3\, ky\right)\right]\right)$

In[44]:=
```
FullSimplify[2 Cos[1/2 a (Sqrt[3] kx - 3 ky)] + 2 Cos[1/2 a (Sqrt[3] kx + 3 ky)]]
```

Out[44]= $2 \left(\cos\left[\frac{1}{2} a \left(\sqrt{3}\, kx - 3\, ky\right)\right] + \cos\left[\frac{1}{2} a \left(\sqrt{3}\, kx + 3\, ky\right)\right]\right)$

In[49]:=
```
Expand[Cos[1/2 a (Sqrt[3] kx - 3 ky)] + Cos[1/2 a (Sqrt[3] kx + 3 ky)]]
```

Out[49]= $\cos\left[\frac{1}{2} a \left(\sqrt{3}\, kx - 3\, ky\right)\right] + \cos\left[\frac{1}{2} a \left(\sqrt{3}\, kx + 3\, ky\right)\right]$

In[53]:=
```
2 * Pi / Sqrt[3.]
```

Out[53]= 3.6276

Finding band touching points

In[62]:=
```
1 + 4 * (Cos[Sqrt[3] / 2 * a * kx]) ^2 / (-4 * Cos[a / 2 * Sqrt[3] * kx])
```

Out[62]= $1 - \cos\left[\frac{1}{2} \sqrt{3}\, a\, kx\right]$

In[67]:=
```
Pi / Sqrt[3.]
```

Out[67]= 1.8138

In[81]:=
```
Δ = Simplify[
  Exp[I * Dot[k, a1]] + Exp[I * Dot[k, a2]] + Exp[I * Dot[k, a3]] /. kx → Kx + qx /. ky → Ky + qy]
```

Out[81]= $e^{-\frac{1}{2} i a \left(-Ky + \sqrt{3}\, (Kx + qx) - qy\right)} + e^{-i a (Ky + qy)} + e^{\frac{1}{2} i a \left(Ky + \sqrt{3}\, (Kx + qx) + qy\right)}$

In[78]:=
```
FullSimplify[Series[Δ, {qx, 0, 2}, {qy, 0, 2}]]
```

Out[78]= $\left(\left(e^{-\frac{1}{2} i a \left(\sqrt{3}\, Kx - Ky\right)} + e^{-i a Ky} + e^{\frac{1}{2} i a \left(\sqrt{3}\, Kx + Ky\right)}\right) + \frac{1}{2} i a \left(e^{-\frac{1}{2} i a \left(\sqrt{3}\, Kx - Ky\right)} - 2 e^{-i a Ky} + e^{\frac{1}{2} i a \left(\sqrt{3}\, Kx + Ky\right)}\right) qy + \frac{1}{8} a^2 \left(-e^{-\frac{1}{2} i a \left(\sqrt{3}\, Kx - Ky\right)} - 4 e^{-i a Ky} - e^{\frac{1}{2} i a \left(\sqrt{3}\, Kx + Ky\right)}\right) qy^2 + O[qy]^3\right) + \left(-\sqrt{3}\, a\, e^{\frac{i a Ky}{2}} \sin\left[\frac{1}{2} \sqrt{3}\, a\, Kx\right] - \frac{1}{2} i \sqrt{3}\, a^2 e^{\frac{i a Ky}{2}} \sin\left[\frac{1}{2} \sqrt{3}\, a\, Kx\right] qy + \frac{1}{8} \sqrt{3}\, a^3 e^{\frac{i a Ky}{2}} \sin\left[\frac{1}{2} \sqrt{3}\, a\, Kx\right] qy^2 + O[qy]^3\right) qx + \left(-\frac{3}{4} \left(a^2 e^{\frac{i a Ky}{2}} \cos\left[\frac{1}{2} \sqrt{3}\, a\, Kx\right]\right) - \frac{3}{8} i a^3 e^{\frac{i a Ky}{2}} \cos\left[\frac{1}{2} \sqrt{3}\, a\, Kx\right] qy + \frac{3}{32} a^4 e^{\frac{i a Ky}{2}} \cos\left[\frac{1}{2} \sqrt{3}\, a\, Kx\right] qy^2 + O[qy]^3\right) qx^2 + O[qx]^3$

In[86]:=
```
Simplify[Series[Series[Δ, {qx, 0, 1}], {qy, 0, 1}]]
```

Out[86]=
$$\left(\left(e^{-\frac{1}{2}\,i\,a\left(\sqrt{3}\,Kx-Ky\right)}+e^{-i\,a\,Ky}+e^{\frac{1}{2}\,i\,a\left(\sqrt{3}\,Kx+Ky\right)}\right)+\frac{1}{2}\,i\,a\left(e^{-\frac{1}{2}\,i\,a\left(\sqrt{3}\,Kx-Ky\right)}-2\,e^{-i\,a\,Ky}+e^{\frac{1}{2}\,i\,a\left(\sqrt{3}\,Kx+Ky\right)}\right)qy+O[qy]^2\right)+\left(\frac{1}{2}\,i\,\sqrt{3}\,a\,e^{-\frac{1}{2}\,i\,a\left(\sqrt{3}\,Kx-Ky\right)}\left(-1+e^{i\sqrt{3}\,a\,Kx}\right)-\frac{1}{4}\left(\sqrt{3}\,a^2\,e^{-\frac{1}{2}\,i\,a\left(\sqrt{3}\,Kx-Ky\right)}\left(-1+e^{i\sqrt{3}\,a\,Kx}\right)\right)qy+O[qy]^2\right)qx+O[qx]^2$$

In[88]:=
```
ArcCos[1/2]
```

Out[88]=
$$\frac{\pi}{3}$$

In[89]:=
```
M = Exp[I * a * ky/2] * (2 * Cos[a * kx * Sqrt[3]/2] + Exp[-I * 3 * a * ky/2])
```

Out[89]=
$$e^{\frac{i\,a\,ky}{2}}\left(e^{-\frac{3}{2}\,i\,a\,ky}+2\,\text{Cos}\left[\frac{1}{2}\sqrt{3}\,a\,kx\right]\right)$$

In[92]:=
```
Kx = 2 * Pi/a * (1/(3 * Sqrt[3]))
```

Out[92]=
$$\frac{2\,\pi}{3\sqrt{3}\,a}$$

In[93]:=
```
Ky = 2 * Pi/a * (1/(3))
```

Out[93]=
$$\frac{2\,\pi}{3\,a}$$

In[96]:=
```
Kxp = -Kx
```

Out[96]=
$$-\frac{2\,\pi}{3\sqrt{3}\,a}$$

In[97]:=
```
Kyp = Ky
```

Out[97]=
$$\frac{2\,\pi}{3\,a}$$

In[94]:=
```
D[M, kx] /. {kx → Kx, ky → Ky}
```

Out[94]=
$$-\frac{3}{2}\,a\,e^{\frac{i\,\pi}{3}}$$

In[95]:=
```
D[M, ky] /. {kx → Kx, ky → Ky}
```

Out[95]=
$$-\frac{3}{2}\,i\,a\,e^{-\frac{2\,i\,\pi}{3}}$$

In[98]:=
```
D[M, kx] /. {kx → Kxp, ky → Kyp}
```

Out[98]=
$$\frac{3}{2}\,a\,e^{\frac{i\,\pi}{3}}$$

In[99]:=
```
D[M, ky] /. {kx → Kxp, ky → Kyp}
```

Out[99]=
$$-\frac{3}{2}\,i\,a\,e^{-\frac{2\,i\,\pi}{3}}$$