

```

Γ0 = {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}};
Γ1 = {{0, 1, 0}, {1, 0, 0}, {0, 0, 0}};
Γ3 = {{1, 0, 0}, {0, -1, 0}, {0, 0, 0}};
Γ4 = {{0, 0, 1}, {0, 0, 0}, {1, 0, 0}};
Γ6 = {{0, 0, 0}, {0, 0, 1}, {0, 1, 0}};
Γ8 = 1 / Sqrt[3] {{1, 0, 0}, {0, 1, 0}, {0, 0, -2}};
h = {h0, h1, h3, h4, h6, h8}.{Γ0, Γ1, Γ3, Γ4, Γ6, Γ8};

h0 = 0

In[1831]:= Nx = 3;
Ny = 3;
nx = Table[i, {i, -Nx, Nx}];
ny = Table[j, {j, -Ny, Ny}];
Nnx = Dimensions[nx][[1]];
Nny = Dimensions[ny][[1]];

hj =
Sum[Exp[I π {kx, ky}.{nx[[ix]], ny[[iy]]}] tj[ix, iy], {ix, 1, Nnx}, {iy, 1, Nny}]

Out[1837]= e^(i (-3 kx-3 ky) π) tj[1, 1] + e^(i (-3 kx-2 ky) π) tj[1, 2] + e^(i (-3 kx-ky) π) tj[1, 3] + e^(-3 i kx π) tj[1, 4] +
e^(i (-3 kx+ky) π) tj[1, 5] + e^(i (-3 kx+2 ky) π) tj[1, 6] + e^(i (-3 kx+3 ky) π) tj[1, 7] +
e^(i (-2 kx-3 ky) π) tj[2, 1] + e^(i (-2 kx-2 ky) π) tj[2, 2] + e^(i (-2 kx-ky) π) tj[2, 3] + e^(-2 i kx π) tj[2, 4] +
e^(i (-2 kx+ky) π) tj[2, 5] + e^(i (-2 kx+2 ky) π) tj[2, 6] + e^(i (-2 kx+3 ky) π) tj[2, 7] +
e^(i (-kx-3 ky) π) tj[3, 1] + e^(i (-kx-2 ky) π) tj[3, 2] + e^(i (-kx-ky) π) tj[3, 3] + e^(-i kx π) tj[3, 4] +
e^(i (-kx+ky) π) tj[3, 5] + e^(i (-kx+2 ky) π) tj[3, 6] + e^(i (-kx+3 ky) π) tj[3, 7] + e^(-3 i ky π) tj[4, 1] +
e^(-2 i ky π) tj[4, 2] + e^(-i ky π) tj[4, 3] + tj[4, 4] + e^(i ky π) tj[4, 5] + e^(2 i ky π) tj[4, 6] +
e^(3 i ky π) tj[4, 7] + e^(i (kx-3 ky) π) tj[5, 1] + e^(i (kx-2 ky) π) tj[5, 2] + e^(i (kx-ky) π) tj[5, 3] +
e^(i kx π) tj[5, 4] + e^(i (kx+ky) π) tj[5, 5] + e^(i (kx+2 ky) π) tj[5, 6] + e^(i (kx+3 ky) π) tj[5, 7] +
e^(i (2 kx-3 ky) π) tj[6, 1] + e^(i (2 kx-2 ky) π) tj[6, 2] + e^(i (2 kx-ky) π) tj[6, 3] +
e^(2 i kx π) tj[6, 4] + e^(i (2 kx+ky) π) tj[6, 5] + e^(i (2 kx+2 ky) π) tj[6, 6] + e^(i (2 kx+3 ky) π) tj[6, 7] +
e^(i (3 kx-3 ky) π) tj[7, 1] + e^(i (3 kx-2 ky) π) tj[7, 2] + e^(i (3 kx-ky) π) tj[7, 3] +
e^(3 i kx π) tj[7, 4] + e^(i (3 kx+ky) π) tj[7, 5] + e^(i (3 kx+2 ky) π) tj[7, 6] + e^(i (3 kx+3 ky) π) tj[7, 7]

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Numerical values of the tight – binding parameters

```
In[1382]:= Chop[t1]
Chop[t3]
Chop[t4]
Chop[t6]
Chop[t8]

Out[1382]= {{0, -0.0626378 + 0.00373984 i, -0.113747 + 0.0240204 i, 0. + 0.0000660094 i,
0.113747 - 0.0241524 i, 0.0626378 - 0.00360782 i, 0. - 0.000132019 i},
{0.0626378 - 0.00373984 i, 0, -0.0421371 - 0.0277602 i, 0. + 0.00367383 i,
0.0421371 + 0.0204126 i, 0. + 0.00734766 i, -0.0626378 - 0.00360782 i},
{0.113747 - 0.0240204 i, 0.0421371 + 0.0277602 i, 0, 0. + 0.0240864 i,
0. - 0.0481728 i, -0.0421371 + 0.0204126 i, -0.113747 - 0.0241524 i},
{0. - 0.0000660094 i, 0. - 0.00367383 i, 0. - 0.0240864 i, 0,
0. + 0.0240864 i, 0. + 0.00367383 i, 0. + 0.0000660094 i},
{-0.113747 + 0.0241524 i, -0.0421371 - 0.0204126 i, 0. + 0.0481728 i,
0. - 0.0240864 i, 0, 0.0421371 - 0.0277602 i, 0.113747 + 0.0240204 i},
{-0.0626378 + 0.00360782 i, 0. - 0.00734766 i, 0.0421371 - 0.0204126 i,
0. - 0.00367383 i, -0.0421371 + 0.0277602 i, 0, 0.0626378 + 0.00373984 i},
{0. + 0.000132019 i, 0.0626378 + 0.00360782 i, 0.113747 + 0.0241524 i,
0. - 0.0000660094 i, -0.113747 - 0.0240204 i, -0.0626378 - 0.00373984 i, 0} }

Out[1383]= {{0.0297665, 0.012528, -0.0431533, -0.0432153, -0.0431533, 0.012528, 0.0297665},
{0.012528, 0.165214, 0.0549507, -0.0753167, 0.0549507, 0.165214, 0.012528},
{-0.0431533, 0.0549507, -0.108615, 0.0600891, -0.108615, 0.0549507, -0.0431533},
{-0.0432153, -0.0753167, 0.0600891,
0.00729899, 0.0600891, -0.0753167, -0.0432153},
{-0.0431533, 0.0549507, -0.108615, 0.0600891, -0.108615, 0.0549507, -0.0431533},
{0.012528, 0.165214, 0.0549507, -0.0753167, 0.0549507, 0.165214, 0.012528},
{0.0297665, 0.012528, -0.0431533, -0.0432153, -0.0431533, 0.012528, 0.0297665} }

Out[1384]= {{0, 0.0530598, 0.148045, 0.199493, 0.148045, 0.0530598, 0},
{-0.0530598, 0, 0.065518, 0.0839606, 0.065518, 0, -0.0530598},
{-0.148045, -0.065518, 0, -0.312349, 0, -0.065518, -0.148045},
{-0.199493, -0.0839606, 0.312349, 0, 0.312349, -0.0839606, -0.199493},
{-0.148045, -0.065518, 0, -0.312349, 0, -0.065518, -0.148045},
{-0.0530598, 0, 0.065518, 0.0839606, 0.065518, 0, -0.0530598},
{0, 0.0530598, 0.148045, 0.199493, 0.148045, 0.0530598, 0} }

Out[1385]= {{0.0507663, 0.0735257, -0.0489735, 0, 0.0489735, -0.0735257, -0.0507663},
{0.0735257, 0.1579, 0.295589, 0, -0.295589, -0.1579, -0.0735257},
{-0.0489735, 0.295589, -0.249347, 0, 0.249347, -0.295589, 0.0489735},
{0, 0, 0, 0, 0, 0},
{0.0489735, -0.295589, 0.249347, 0, -0.249347, 0.295589, -0.0489735},
{-0.0735257, -0.1579, -0.295589, 0, 0.295589, 0.1579, 0.0735257},
{-0.0507663, -0.0735257, 0.0489735, 0, -0.0489735, 0.0735257, 0.0507663} }

Out[1386]= {{0, 0.0461421, 0, -0.114789, 0, 0.0461421, 0},
{0.0461421, 0, 0.187857, 0.433013, 0.187857, 0, 0.0461421},
{0, 0.187857, 0, -0.30825, 0, 0.187857, 0},
{-0.114789, 0.433013, -0.30825, 0, -0.30825, 0.433013, -0.114789},
{0, 0.187857, 0, -0.30825, 0, 0.187857, 0},
{0.0461421, 0, 0.187857, 0.433013, 0.187857, 0, 0.0461421},
{0, 0.0461421, 0, -0.114789, 0, 0.0461421, 0}}
```

**ACTIVATE FROM HERE
(def of TB paramters,
def Hamiltonian, band structure)**

```
In[1388]:= Nx = 3;
Ny = 3;
nx = Table[i, {i, -Nx, Nx}];
ny = Table[j, {j, -Ny, Ny}];
Nnx = Dimensions[nx][[1]];
Nny = Dimensions[ny][[1]];
h1N = Sum[Exp[I π {kx, ky}.{nx[[ix]], ny[[iy]]}] t1[[ix, iy]],
{ix, 1, Nnx}, {iy, 1, Nny}];
h3N = Sum[Exp[I π {kx, ky}.{nx[[ix]], ny[[iy]]}] t3[[ix, iy]],
{ix, 1, Nnx}, {iy, 1, Nny}];
h4N = Sum[Exp[I π {kx, ky}.{nx[[ix]], ny[[iy]]}] t4[[ix, iy]],
{ix, 1, Nnx}, {iy, 1, Nny}];
h6N = Sum[Exp[I π {kx, ky}.{nx[[ix]], ny[[iy]]}] t6[[ix, iy]],
{ix, 1, Nnx}, {iy, 1, Nny}];
h8N = Sum[Exp[I π {kx, ky}.{nx[[ix]], ny[[iy]]}] t8[[ix, iy]],
{ix, 1, Nnx}, {iy, 1, Nny}];

In[1399]:= Nk = 40;
{Aa, Bb, Cc, Dd} = {-1., 1., -1., 1.};
{-0.5, -0.3, -1.1, -0.9};
{-1., 1., -1, 1.};
K1 = Table[i, {i, Aa, Bb, (Bb - Aa) / Nk}];
K2 = Table[i, {i, Cc, Dd, (Dd - Cc) / Nk}];
GMO = {{1, 0, 0}, {0, 1, 0}, {0, 0, 1}};
GM1 = {{0, 1, 0}, {1, 0, 0}, {0, 0, 0}};
GM2 = {{0, -I, 0}, {I, 0, 0}, {0, 0, 0}};
GM3 = {{1, 0, 0}, {0, -1, 0}, {0, 0, 0}};
GM4 = {{0, 0, 1}, {0, 0, 0}, {1, 0, 0}};
GM5 = {{0, 0, -I}, {0, 0, 0}, {I, 0, 0}};
GM6 = {{0, 0, 0}, {0, 0, 1}, {0, 1, 0}};
GM7 = {{0, 0, 0}, {0, 0, -I}, {0, I, 0}};
GM8 = 1 / Sqrt[3] {{1, 0, 0}, {0, 1, 0}, {0, 0, -2}};
HFn = {0, h1N, h3N, h4N, h6N, h8N}.{GMO, GM1, GM3, GM4, GM6, GM8};

En = Table[Sort[Re[Eigenvalues[N[HFn /. {kx → K1[[i]], ky → K2[[j]]}]]]],
{i, 1, Dimensions[K1][[1]]}, {j, 1, Dimensions[K2][[1]]}];
ListPlot3D[Table[Transpose[En[[;;, ;, i]]], {i, 1, 3}],
InterpolationOrder → 1, AxesLabel → {"kx", "ky", "E"}, ImageSize → 500,
DataRange → {{Aa, Bb}, {Cc, Dd}}, PlotStyle → {Opacity[0.8]}]
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