

Staggered chemical potential and the surface bands of Sr_2RuO_4

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In this notebook we will examine the effect of a staggered chemical potential on the dispersion of the surface bands of Sr_2RuO_4 . We will focus in particular on the M point. The staggered chemical potential breaks the lattice reflection symmetry but preserves the fourfold rotation symmetry about each Ru atom. As we will see below, this allows the two d_{xy} bands at the M point to decouple and become individually four-fold symmetric. This allows the bands to host X_9 singularities under tuning.

Loading the Library

We first load the library by executing the following:

```
In[ ]:= AppendTo[$Path, StringDelete[NotebookDirectory[], "/Sr2RuO4"] <> "Package"];  
<< BandUtilities`
```

Interpolating between the Wannier90 files

Ingredients needed for symmetrization

```
In[ ]:= ρ = {{0, -1, 0}, {1, 0, 0}, {0, 0, 1}};
(*The matrix part of the C4 rotation about one of the Ru atoms.*)
Uρ = {{0, -1, 0}, {1, 0, 0}, {0, 0, -1}};
(*Representation of C4 rotation in the d-orbital space.*)

rxy = {{0, 1, 0}, {1, 0, 0}, {0, 0, 1}}; (*x↔y reflection.*)
Urxy = {{-1, 0, 0}, {0, 1, 0}, {0, 0, -1}};
(*Representation of the x↔y reflection.*)

c0 = {1/4, 3/4, 0}; (*Location of one of the Ru atoms,
which we shall use as the centre of the C4 rotation.*)

AtomLocations =
  {{3/4, 1/4, 0}, {3/4, 1/4, 0}, {3/4, 1/4, 0}, {1/4, 3/4, 0}, {1/4, 3/4, 0}, {1/4, 3/4, 0}};
(*Location of the basis atoms in the fractional
coordinates within the unit cell.*)

SymmetryList = {}; (*This is a multidimensional list which we shall
construct below. Each element is a sublist corresponding to a particular
symmetry. First element of the sublist is real space symmetry's matrix part,
second element is the translation part and the third element is
its representation in the Hilbert space. Our point group is D4,
or D8 in some people's notation.*)
Do[
  AppendTo[SymmetryList,
    {MatrixPower[ρ, i], (c0 - MatrixPower[ρ, i].c0) // Simplify,
    ArrayFlatten[IdentityMatrix[2]⊗MatrixPower[Uρ, i]]}];

  AppendTo[SymmetryList,
    {MatrixPower[ρ, i].rxy, (c0 - MatrixPower[ρ, i].c0) // Simplify,
    ArrayFlatten[IdentityMatrix[2]⊗MatrixPower[Uρ, i]].
    ArrayFlatten[{{0, 1}, {1, 0}}⊗Urxy]}];
  , {i, 1, 4}];
```

Interpolation with symmetrization

We now interpolate between the Wannier90 data for 13 different rotations of the RuO octahedra: 0° through 12° to generate a continuously θ dependent Hamiltonian, whilst ensuring that the interpolated model has the right symmetry (for which we are feeding the list SymmetryList):

```
In[ ]:= FileLocn = NotebookDirectory[] <> "unrenormalized2/";
```

```
W90Data = LoadInterpolateTBMs[{FileLocn <> "Sr2Ru04_0deg.dat",
  FileLocn <> "Sr2Ru04_1deg.dat", FileLocn <> "Sr2Ru04_2deg.dat",
  FileLocn <> "Sr2Ru04_3deg.dat", FileLocn <> "Sr2Ru04_4deg.dat",
  FileLocn <> "Sr2Ru04_5deg.dat", FileLocn <> "Sr2Ru04_6deg.dat",
  FileLocn <> "Sr2Ru04_7deg.dat", FileLocn <> "Sr2Ru04_8deg.dat",
  FileLocn <> "Sr2Ru04_9deg.dat", FileLocn <> "Sr2Ru04_10deg.dat",
  FileLocn <> "Sr2Ru04_11deg.dat", FileLocn <> "Sr2Ru04_12deg.dat"},
{0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12}, "Symmetries" → SymmetryList,
"OrbitalCentres" → AtomLocations, "ParameterSymbol" → "θ"];
```

Invalid or no lattice vectors provided! Using unit vectors.

Tight-binding data files loaded.

Space dimension: 3

Number of orbitals: 6

Number of supercells: 49

Number of models/data-files to interpolate: 13

Number of lines in the data files:

```
{741, 853, 853, 853, 845, 853, 853, 853, 853, 853, 853, 853, 853}
```

Interpolating between the Hamiltonians.

Valid symmetrization scheme provided! We will symmetrize the loaded Hamiltonian.

Number of supercells after symmetrization: 79

Since this is largely an exploratory analysis, we will not include the overall band renormalization or the spin orbit term which have minimal impact on the M point. We begin by adding a staggered chemical potential Δ

```
In[270]:= Hamltn1[k1_, k2_, θ_, Δ_] = W90Data[[1]] + DiagonalMatrix[{Δ, Δ, Δ, -Δ, -Δ, -Δ}];
```

Tuning to a HOS with non - zero Δ

We begin by defining a version of the Hamiltonian suitable for series expansion (once again in the bulk Brillouin zone basis for the sake of consistency)

```
In[271]:= Ham[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]], k[[3]], k[[4]]
```

To compute the Hessian determinant with $\delta\theta$ and $\delta\Delta$ corrections, we need to series expand the dispersion to quadratic order with corrections. To find the bands closest to Fermi level to series expand, we first calculate the eigenvalues at the M point for a small $\Delta=0.005$ (that is 5 meV).

```
In[272]:= Sort[Eigenvalues[Ham[{0, π // N, 8, 0.005}]]]
```

```
Out[272]:= {-0.555813, -0.555813, -0.076319, -0.066319, 0.286847, 0.286847}
```

It is clear that bands 3 and 4 are the bands of interest closest to the Fermi level. We will plot these bands with orbital projection once the critical θ has been figured out.

Band 3

```
In[273]:= TaylA = Chop[TaylorExpandBand[Ham,
    {0,  $\pi$  // N, 8, 0.005}, 3, 2, "Dimension" → 2, "TuningDegree" → 2,
    "TuningSymbol" → {" $\delta\theta$ ", " $\delta\Delta$ "}, "Messages" → False][[1], 10-8];
```

```
In[277]:= Chop[Total[TaylA]] /. {p1 → kx, p2 → ky}
```

```
Out[277]= -0.076319 - 1.  $\delta\Delta$  + (-0.0205955 + 0.00119685  $\delta\theta$ )  $\delta\theta$  +
    (-0.014985 + 8.34065 × 10-8  $\delta\Delta^2$  + (0.0320869 - 0.000243806  $\delta\theta$ )  $\delta\theta$ ) kx2 +
    (-0.014985 - 8.34065 × 10-8  $\delta\Delta^2$  + (0.0320869 - 0.000243806  $\delta\theta$ )  $\delta\theta$ ) ky2
```

We note that the quadratic term contains a very small $\delta\Delta$ correction. This indicates that the critical θ does not depend strongly on Δ (as long as it is non-zero and small. For large Δ , this analysis based on series expansion to quadratic order may not hold).

We can compute the Hessian determinant and solve for $\delta\theta$ by setting it to zero:

```
In[278]:= HesDet = ((D[TaylA][[3]], {p1, 2}) × D[TaylA][[3]], {p2, 2}]) - (D[TaylA][[3]], p1, p2))2) /.
    {p1 → 0, p2 → 0,  $\delta\lambda$  → 0,  $\delta\Delta$  → 0} // Simplify
Soln1 = Solve[HesDet == 0,  $\delta\theta$ ]
```

```
Out[278]= 0.000898201 - 0.00384658  $\delta\theta$  + 0.00414751  $\delta\theta^2$  - 0.000062584  $\delta\theta^3$  + 2.37766 × 10-7  $\delta\theta^4$ 
```

```
Out[279]= {{ $\delta\theta$  → 0.468682}, { $\delta\theta$  → 0.468682}, { $\delta\theta$  → 131.14}, { $\delta\theta$  → 131.14}}
```

The critical θ to the first approximation is then given by

```
In[280]:= TaylB = Chop[TaylorExpandBand[Ham, {0,  $\pi$  // N, 8 +  $\delta\theta$  /. Soln1[[1]], 0.005},
    3, 2, "Dimension" → 2, "TuningDegree" → 2,
    "TuningSymbol" → {" $\delta\theta$ ", " $\delta\Delta$ "}, "Messages" → False][[1], 10-8];
```

```
In[*]:= Total[TaylB] /. {p1 → kx, p2 → ky}
```

```
Out[*]= -0.0856538 - 1.  $\delta\Delta$  + (-0.0191726 + 0.00162093  $\delta\theta$ )  $\delta\theta$  +
    (0.0000166482 - 3.94981 × 10-8  $\delta\Delta^2$  + (0.0319471 - 0.000137449  $\delta\theta$ )  $\delta\theta$ ) kx2 +
    (0.0000166482 + 3.94981 × 10-8  $\delta\Delta^2$  + (0.0319471 - 0.000137449  $\delta\theta$ )  $\delta\theta$ ) ky2
```

Indeed the coefficients of the quadratic terms have become quite small. We can repeat the process once again to obtain better convergence

```
In[281]:= HesDet = ((D[TaylB][[3]], {p1, 2}) × D[TaylB][[3]], {p2, 2}]) - (D[TaylB][[3]], p1, p2))2) /.
    {p1 → 0, p2 → 0,  $\delta\lambda$  → 0,  $\delta\Delta$  → 0} // Simplify
Soln2 = Solve[HesDet == 0,  $\delta\theta$ ]
```

```
Out[281]= 1.10864 × 10-9 + 4.25488 × 10-6  $\delta\theta$  + 0.00408246  $\delta\theta^2$  - 0.0000351289  $\delta\theta^3$  + 7.55692 × 10-8  $\delta\theta^4$ 
```

```
Out[282]= {{ $\delta\theta$  → -0.000521115}, { $\delta\theta$  → -0.000521115}, { $\delta\theta$  → 232.429}, { $\delta\theta$  → 232.429}}
```

Thus, the critical theta is given by

```
In[283]:=  $\theta_{crit}$  = 8 + ( $\delta\theta$  /. Soln1[[1]]) + ( $\delta\theta$  /. Soln2[[1]])
```

```
Out[283]= 8.46816
```

Using this, we go ahead and define the Hamiltonian at the critical θ :

```
In[284]:= HamCrit[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]],  $\theta_{crit}$ , 0.005]
```

```
In[285]:= TaylC =  
  Chop[TaylorExpandBand[HamCrit, {0,  $\pi$  // N}, 3, 4, "Messages" → False][[1]],  $10^{-8}$ ];
```

```
In[286]:= Total[TaylC] /. {p1 →  $k_x$ , p2 →  $k_y$ }
```

```
Out[286]:= -0.0856438 - 0.630949  $k_x^4$  + 0.102619  $k_x^3 k_y$  + 0.860439  $k_x^2 k_y^2$  - 0.102619  $k_x k_y^3$  - 0.630949  $k_y^4$ 
```

This is obviously a singularity belonging to the X_9 class. We can confirm this explicitly

```
In[287]:= DiagnoseHOS[Total[TaylC] /. {p1 →  $k_x$ , p2 →  $k_y$ }]
```

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4 and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

```
Out[287]:= {2, 8, 5}
```

We can also explicitly check that this satisfies the four fold rotation symmetry $(k_x, k_y) \rightarrow (k_y, -k_x)$ but not the mirror symmetry $(k_x, k_y) \rightarrow (k_y, k_x)$ since the latter is broken while the former is preserved under the staggered chemical potential Δ .

```
In[288]:= Chop[(Total[TaylC /. {p1 →  $k_x$ , p2 →  $k_y$ }] - Total[TaylC /. {p1 →  $k_y$ , p2 → - $k_x$ }]) // FullSimplify,  
   $10^{-6}$ ] // Total
```

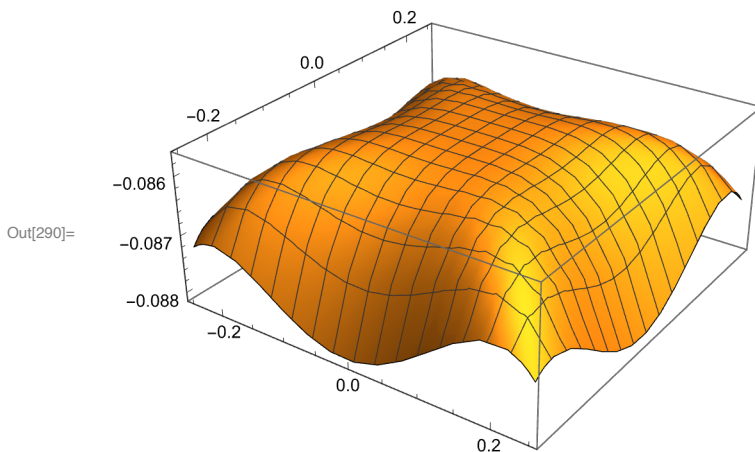
```
Chop[(Total[TaylC /. {p1 →  $k_x$ , p2 →  $k_y$ }] - Total[TaylC /. {p1 →  $k_y$ , p2 →  $k_x$ }]) // FullSimplify,  
   $10^{-6}$ ] // Total
```

```
Out[288]:= 0
```

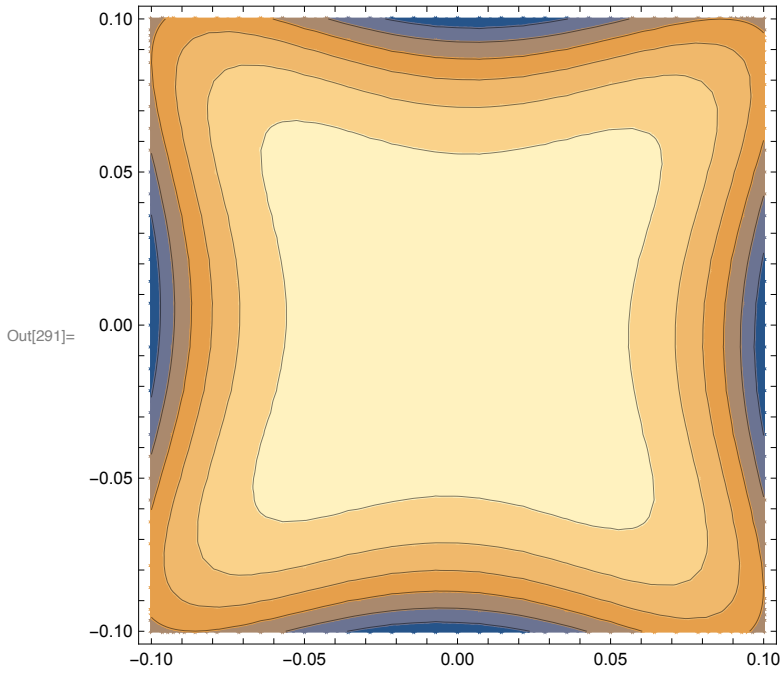
```
Out[289]:= 0.205239  $k_x^3 k_y$  - 0.205239  $k_x k_y^3$ 
```

The 3D and surface plot of the dispersion

```
In[290]:= Plot3D[Total[TaylC], {p1,  $-\frac{1}{4}$ ,  $\frac{1}{4}$ }, {p2,  $-\frac{1}{4}$ ,  $\frac{1}{4}$ }]
```



```
In[291]:= ContourPlot[Total[TaylC], {p1,  $-\frac{1}{10}, \frac{1}{10}$ }, {p2,  $-\frac{1}{10}, \frac{1}{10}$ }]
```



These indicate that this is a four fold maximum rather than a saddle.

Band 4

```
In[292]:= TaylA2 = Chop[TaylorExpandBand[Ham,
    {0,  $\pi$  // N, 8, 0.005}, 4, 2, "Dimension" → 2, "TuningDegree" → 2,
    "TuningSymbol" → {" $\delta\theta$ ", " $\delta\Delta$ "}, "Messages" → False][[1], 10-8];
```

```
In[293]:= Total[TaylA2] /. {p1 → kx, p2 → ky}
```

```
Out[293]= -0.066319 + 1.  $\delta\Delta$  + (-0.0205955 + 0.00119685  $\delta\theta$ )  $\delta\theta$  +
    (-0.014985 - 8.34065 × 10-8  $\delta\Delta^2$  + (0.0320869 - 0.000243806  $\delta\theta$ )  $\delta\theta$ ) kx2 +
    (-0.014985 + 8.34065 × 10-8  $\delta\Delta^2$  + (0.0320869 - 0.000243806  $\delta\theta$ )  $\delta\theta$ ) ky2
```

We note that the quadratic term contains a very small $\delta\Delta$ correction. This indicates that the critical θ does not depend strongly on Δ (as long as it is non-zero and small. For large Δ , this analysis based on series expansion to quadratic order may not hold).

We can compute the Hessian determinant and solve for $\delta\theta$ by setting it to zero:

```
In[294]:= HesDet =
    ((D[TaylA2[[3]], {p1, 2}] × D[TaylA2[[3]], {p2, 2}]) - (D[TaylA2[[3]], p1, p2])2) /.
    {p1 → 0, p2 → 0,  $\delta\lambda$  → 0,  $\delta\Delta$  → 0} // Simplify
    Soln12 = Solve[HesDet == 0,  $\delta\theta$ ]
```

```
Out[294]= 0.000898201 - 0.00384658  $\delta\theta$  + 0.00414751  $\delta\theta^2$  - 0.000062584  $\delta\theta^3$  + 2.37766 × 10-7  $\delta\theta^4$ 
```

```
Out[295]= {{ $\delta\theta$  → 0.468682}, { $\delta\theta$  → 0.468682}, { $\delta\theta$  → 131.14}, { $\delta\theta$  → 131.14}}
```

The critical θ to the first approximation is then given by

```
In[296]:= TaylB2 = Chop[TaylorExpandBand[Ham, {0,  $\pi$  // N, 8 +  $\delta\theta$  /. Soln12[[1]], 0.005},
  4, 2, "Dimension" → 2, "TuningDegree" → 2,
  "TuningSymbol" → {" $\delta\theta$ ", " $\delta\Delta$ "}, "Messages" → False][[1], 10-8];
```

```
In[297]:= Total[TaylB2] /. {p1 → kx, p2 → ky}
```

```
Out[297]:= -0.0756538 + 1.  $\delta\Delta$  + (-0.0191726 + 0.00162093  $\delta\theta$ )  $\delta\theta$  +
  (0.0000166482 - 9.02946 × 10-8  $\delta\Delta^2$  + (0.0319471 - 0.000137449  $\delta\theta$ )  $\delta\theta$ ) kx2 +
  (0.0000166482 + 9.02946 × 10-8  $\delta\Delta^2$  + (0.0319471 - 0.000137449  $\delta\theta$ )  $\delta\theta$ ) ky2
```

Indeed the coefficients of the quadratic terms have become quite small. We can repeat the process once again to obtain better convergence

```
In[298]:= HesDet =
  ((D[TaylB2[[3]], {p1, 2}] × D[TaylB2[[3]], {p2, 2}]) - (D[TaylB2[[3]], p1, p2])2) /.
  {p1 → 0, p2 → 0,  $\delta\lambda$  → 0,  $\delta\Delta$  → 0} // Simplify
Soln22 = Solve[HesDet == 0,  $\delta\theta$ ]
```

```
Out[298]:= 1.10864 × 10-9 + 4.25488 × 10-6  $\delta\theta$  + 0.00408246  $\delta\theta^2$  - 0.0000351289  $\delta\theta^3$  + 7.55692 × 10-8  $\delta\theta^4$ 
```

```
Out[299]:= {{ $\delta\theta$  → -0.000521115}, { $\delta\theta$  → -0.000521115}, { $\delta\theta$  → 232.429}, { $\delta\theta$  → 232.429}}
```

Thus, the critical theta is given by

```
In[300]:=  $\theta_{crit2}$  = 8 + ( $\delta\theta$  /. Soln12[[1]]) + ( $\delta\theta$  /. Soln22[[1]])
```

```
Out[300]:= 8.46816
```

Using this, we go ahead and define the Hamiltonian at the critical θ :

```
In[301]:= HamCrit2[k_] := Ham1tn1[k[[1]] - k[[2]], k[[1]] + k[[2]],  $\theta_{crit2}$ , 0.005]
```

```
In[302]:= TaylC2 =
  Chop[TaylorExpandBand[HamCrit2, {0,  $\pi$  // N}, 4, 4, "Messages" → False][[1], 10-8];
```

```
In[303]:= Total[TaylC2] /. {p1 → kx, p2 → ky}
```

```
Out[303]:= -0.0756438 + 0.201354 kx4 - 0.102619 kx3 ky - 0.804168 kx2 ky2 + 0.102619 kx ky3 + 0.201354 ky4
```

This is obviously a singularity belonging to the X_9 class. We can confirm this explicitly

```
In[304]:= DiagnoseHOS[Total[TaylC2] /. {p1 → kx, p2 → ky}]
```

```
Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
```

```
Polynomial has a catastrophe belonging to the  $X_9$  singularity class.
```

```
Out[304]:= {2, 8, 5}
```

We can also explicitly check that this satisfies the four fold rotation symmetry $(k_x, k_y) \rightarrow (k_y, -k_x)$ but not the mirror symmetry $(k_x, k_y) \rightarrow (k_y, k_x)$ since the latter is broken while the former is preserved under the staggered chemical potential Δ .

```

In[305]:= Chop[ ( (TaylC2 /. {p1 → kx, p2 → ky} ) - (TaylC2 /. {p1 → ky, p2 → -kx} ) ) //
FullSimplify, 10-6] // Total
Chop[ ( (TaylC2 /. {p1 → kx, p2 → ky} ) - (TaylC2 /. {p1 → ky, p2 → kx} ) ) // FullSimplify,
10-6] // Total

```

Out[305]= 0

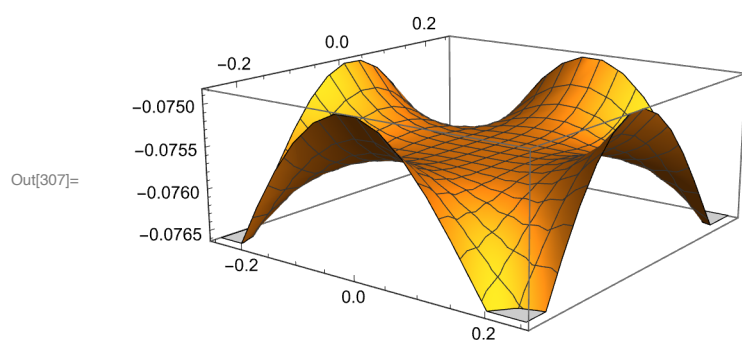
Out[306]= $-0.205239 k_x^3 k_y + 0.205239 k_x k_y^3$

The 3D and surface plot of the dispersion

```

In[307]:= Plot3D[Total[TaylC2], {p1,  $-\frac{1}{4}, \frac{1}{4}$ }, {p2,  $-\frac{1}{4}, \frac{1}{4}$ }]

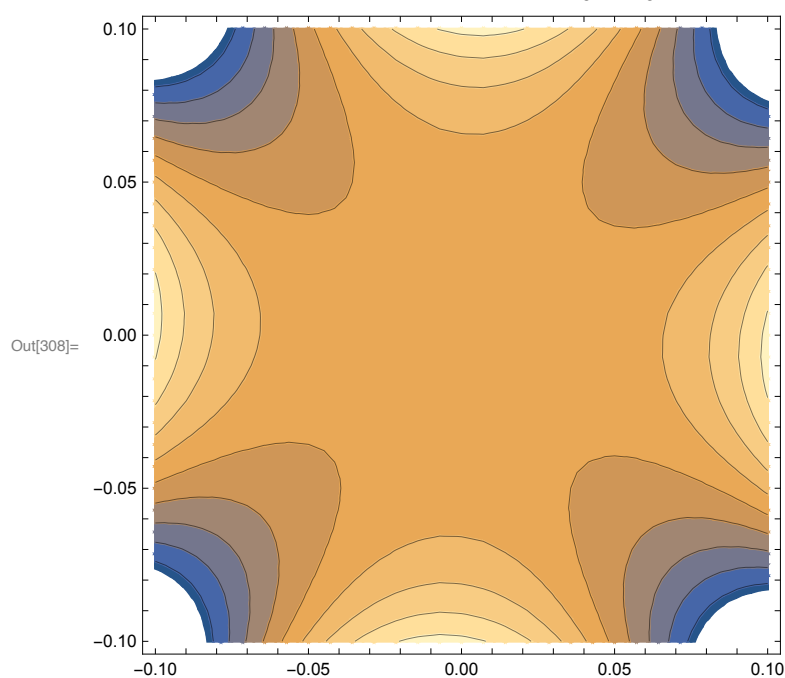
```



```

In[308]:= ContourPlot[Total[TaylC2], {p1,  $-\frac{1}{10}, \frac{1}{10}$ }, {p2,  $-\frac{1}{10}, \frac{1}{10}$ }]

```



These confirm that this is a genuine four fold saddle.

Comparing bands 3 and 4

We can finally compare the HOS in band 3 and band 4 (recall that these bands were degenerate before the staggered chemical potential was applied)


```
In[309]:= Total[TaylC] /. {p1 → kx, p2 → ky}
          Total[TaylC2] /. {p1 → kx, p2 → ky}
```

```
Out[309]= -0.0856438 - 0.630949 kx4 + 0.102619 kx3 ky + 0.860439 kx2 ky2 - 0.102619 kx ky3 - 0.630949 ky4
```

```
Out[310]= -0.0756438 + 0.201354 kx4 - 0.102619 kx3 ky - 0.804168 kx2 ky2 + 0.102619 kx ky3 + 0.201354 ky4
```

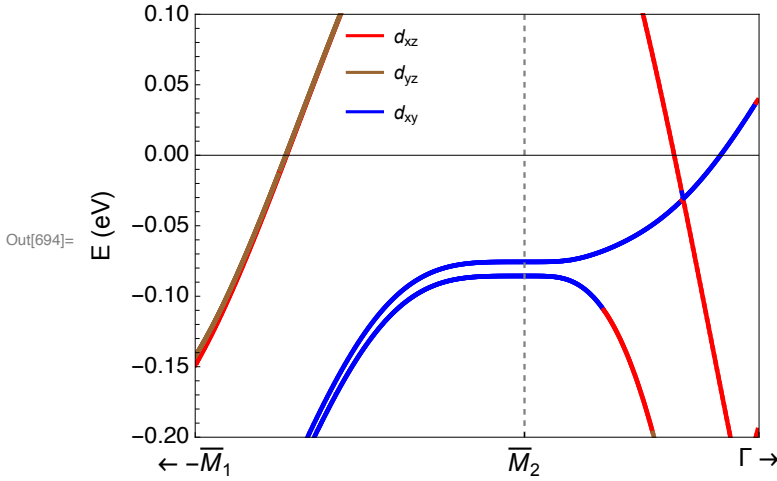
It is clear that while band 3 (with negative k_x^4 and k_y^4 terms) and band 4 (with positive k_x^4 and k_y^4 terms) disperse roughly in the opposite fashion. This is obviously an approximate qualification since the $k_x^2 k_y^2$ terms also play a role. We now plot the band structure with orbital projections

```
δk = 3.869 × 0.35;
```

```
HSymmPts = {{{-δk, π - δk}, "← -M1"}, {{0, π}, "M2"}, {{0, π + δk + 0.01}, "Γ →"}};
```

```
Bnds = GenerateBandStructure[HamCrit, HSymmPts, "OrbitalProjection" → True,
  "OrbitalGrouping" → {{1, 4}, {2, 5}, {3, 6}}, "TotalPoints" → 400];
```

```
In[694]:= PlotBandStructure[Bnds, ({-0.042, 0.012}){-0.2, 0.1}, AspectRatio →  $\frac{3}{4}$ ,
  "yLabel" → {(*Label*)"E (eV)", (*Font Size*)13, (*Font Color*)
    Black, (*Font Family*)"Arial"}, "xLabel" → {13, Black, "Arial"},
  "yTicks" → {12, Black, "Helvetica"}, "LineThickness" → 0.008,
  "LineColorScheme" → {Red, Brown, Blue}, (*Dividing Lines*)"DividingLines" →
    {(*Dashing[...])0.01, (*Color*)Gray, (*Thickness*)0.004},
  (*, Legend*)"PlotKeyLegend" → {{{"dxz", "dyz", "dxy"}, {0.25, 0.85}}}]
```



We notice that the M point singularities arise primarily from the d_{xy} orbitals. Further the higher order saddle nature of band 4 and the higher order maximum nature of band 3 are quite apparent.

Evolution of the critical point

Band 3

```

In[338]:= Do[
  Print[" $\Delta_{\text{stag}}$  = ", Round[1000 Delt], "meV"];

  Do[

    HamCurr[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]],  $\theta$ Curr, Delt];

    TaylorPoly = Chop[Total[
      TaylorExpandBand[HamCurr, {0,  $\pi$  // N}, 3, 2, "Messages"  $\rightarrow$  False][[1]], 10-5];

    HesDet =
      (D[TaylorPoly, {p1, 2}]  $\times$  D[TaylorPoly, {p2, 2}] - (D[TaylorPoly, p1, p2])2) /.
      {p1  $\rightarrow$  0, p2  $\rightarrow$  0} // Simplify;

    Print["\t", " $\theta$  = ",  $\theta$ Curr, ", Tayl = ",
      Chop[NumberForm[TaylorPoly, {4, 3}] /. {p1  $\rightarrow$  kx, p2  $\rightarrow$  ky}, 10-3]];

    , { $\theta$ Curr, 7, 12, 1}];

    , {Delt, 0.001, 0.008, 0.001}];

 $\Delta_{\text{stag}}$  = 1meV
 $\theta$  = 7, Tayl = -0.052 - 0.048 kx2 - 0.048 ky2
 $\theta$  = 8, Tayl = -0.072 - 0.015 kx2 - 0.015 ky2
 $\theta$  = 9, Tayl = -0.091 + 0.017 kx2 + 0.017 ky2
 $\theta$  = 10, Tayl = -0.109 + 0.047 kx2 + 0.047 ky2
 $\theta$  = 11, Tayl = -0.137 + 0.075 kx2 + 0.075 ky2
 $\theta$  = 12, Tayl = -0.149 + 0.096 kx2 + 0.096 ky2

 $\Delta_{\text{stag}}$  = 2meV
 $\theta$  = 7, Tayl = -0.053 - 0.048 kx2 - 0.048 ky2
 $\theta$  = 8, Tayl = -0.073 - 0.015 kx2 - 0.015 ky2
 $\theta$  = 9, Tayl = -0.092 + 0.017 kx2 + 0.017 ky2
 $\theta$  = 10, Tayl = -0.110 + 0.047 kx2 + 0.047 ky2
 $\theta$  = 11, Tayl = -0.138 + 0.075 kx2 + 0.075 ky2
 $\theta$  = 12, Tayl = -0.150 + 0.096 kx2 + 0.096 ky2

```

$$\Delta_{\text{stag}} = 3\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.054 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.074 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.093 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.111 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.139 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.151 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 4\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.055 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.075 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.094 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.112 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.140 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.152 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 5\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.056 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.076 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.095 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.113 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.141 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.153 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 6\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.057 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.077 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.096 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.114 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.142 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.154 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 7\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.058 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.078 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.097 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.115 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.143 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.155 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 8\text{meV}$$

$$\begin{aligned}\theta = 7, \text{ Tayl} &= -0.059 - 0.048 k_x^2 - 0.048 k_y^2 \\ \theta = 8, \text{ Tayl} &= -0.079 - 0.015 k_x^2 - 0.015 k_y^2 \\ \theta = 9, \text{ Tayl} &= -0.098 + 0.017 k_x^2 + 0.017 k_y^2 \\ \theta = 10, \text{ Tayl} &= -0.116 + 0.047 k_x^2 + 0.047 k_y^2 \\ \theta = 11, \text{ Tayl} &= -0.144 + 0.075 k_x^2 + 0.075 k_y^2 \\ \theta = 12, \text{ Tayl} &= -0.156 + 0.096 k_x^2 + 0.096 k_y^2\end{aligned}$$

It is clear from the signs of the k_x^2 and k_y^2 coefficients that the VHS simply transitions from an ordinary maximum to ordinary minimum (somewhere between 8° and 9°). We will find the precise location of the HOVHS below.

Band 4

```
In[339]:= Do[
  Print[" $\Delta_{\text{stag}}$  = ", Round[1000 Delt], "meV"];

  Do[

    HamCurr[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]],  $\theta$ Curr, Delt];

    TaylorPoly = Chop[Total[
      TaylorExpandBand[HamCurr, {0,  $\pi$  // N}, 4, 2, "Messages"  $\rightarrow$  False][[1]], 10-5];

    HesDet =
      (D[TaylorPoly, {p1, 2}]  $\times$  D[TaylorPoly, {p2, 2}] - (D[TaylorPoly, {p1, p2}])2) /.
      {p1  $\rightarrow$  0, p2  $\rightarrow$  0} // Simplify;

    Print["\t", " $\theta$  = ",  $\theta$ Curr, ", Tayl = ",
      Chop[NumberForm[TaylorPoly, {4, 3}] /. {p1  $\rightarrow$   $k_x$ , p2  $\rightarrow$   $k_y$ }, 10-3]];

    , { $\theta$ Curr, 7, 12, 1}];

    , {Delt, 0.001, 0.008, 0.001}];

 $\Delta_{\text{stag}}$  = 1meV

 $\theta = 7, \text{ Tayl} = -0.050 - 0.048 k_x^2 - 0.048 k_y^2$ 
 $\theta = 8, \text{ Tayl} = -0.070 - 0.015 k_x^2 - 0.015 k_y^2$ 
 $\theta = 9, \text{ Tayl} = -0.089 + 0.017 k_x^2 + 0.017 k_y^2$ 
 $\theta = 10, \text{ Tayl} = -0.107 + 0.047 k_x^2 + 0.047 k_y^2$ 
 $\theta = 11, \text{ Tayl} = -0.135 + 0.075 k_x^2 + 0.075 k_y^2$ 
 $\theta = 12, \text{ Tayl} = -0.147 + 0.096 k_x^2 + 0.096 k_y^2$ 
```

$$\Delta_{\text{stag}} = 2\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.049 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.069 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.088 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.106 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.134 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.146 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 3\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.048 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.068 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.087 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.105 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.133 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.145 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 4\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.047 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.067 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.086 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.104 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.132 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.144 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 5\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.046 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.066 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.085 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.103 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.131 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.143 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 6\text{meV}$$

$$\theta = 7, \text{Tayl} = -0.045 - 0.048 k_x^2 - 0.048 k_y^2$$

$$\theta = 8, \text{Tayl} = -0.065 - 0.015 k_x^2 - 0.015 k_y^2$$

$$\theta = 9, \text{Tayl} = -0.084 + 0.017 k_x^2 + 0.017 k_y^2$$

$$\theta = 10, \text{Tayl} = -0.102 + 0.047 k_x^2 + 0.047 k_y^2$$

$$\theta = 11, \text{Tayl} = -0.130 + 0.075 k_x^2 + 0.075 k_y^2$$

$$\theta = 12, \text{Tayl} = -0.142 + 0.096 k_x^2 + 0.096 k_y^2$$

$$\Delta_{\text{stag}} = 7\text{meV}$$

```

 $\theta = 7, \text{Tayl} = -0.044 - 0.048 k_x^2 - 0.048 k_y^2$ 
 $\theta = 8, \text{Tayl} = -0.064 - 0.015 k_x^2 - 0.015 k_y^2$ 
 $\theta = 9, \text{Tayl} = -0.083 + 0.017 k_x^2 + 0.017 k_y^2$ 
 $\theta = 10, \text{Tayl} = -0.101 + 0.047 k_x^2 + 0.047 k_y^2$ 
 $\theta = 11, \text{Tayl} = -0.129 + 0.075 k_x^2 + 0.075 k_y^2$ 
 $\theta = 12, \text{Tayl} = -0.141 + 0.096 k_x^2 + 0.096 k_y^2$ 

 $\Delta_{\text{stag}} = 8\text{meV}$ 

 $\theta = 7, \text{Tayl} = -0.043 - 0.048 k_x^2 - 0.048 k_y^2$ 
 $\theta = 8, \text{Tayl} = -0.063 - 0.015 k_x^2 - 0.015 k_y^2$ 
 $\theta = 9, \text{Tayl} = -0.082 + 0.017 k_x^2 + 0.017 k_y^2$ 
 $\theta = 10, \text{Tayl} = -0.100 + 0.047 k_x^2 + 0.047 k_y^2$ 
 $\theta = 11, \text{Tayl} = -0.128 + 0.075 k_x^2 + 0.075 k_y^2$ 
 $\theta = 12, \text{Tayl} = -0.140 + 0.096 k_x^2 + 0.096 k_y^2$ 

```

Here as well, the VHS simply transitions from an ordinary maximum to ordinary minimum (somewhere between 8° and 9°). We will find the precise location of the HOVHS below.

Thus we see that both the singularities transition from an ordinary maximum to an ordinary minimum probably through a HOVHS somewhere between 8° and 9° . This is not surprising since Δ_{stag} does not break the four fold rotation at the M point, so an ordinary saddle is prohibited when the bands are decoupled.

Nature of the HOS

Band 3

```

In[315]:= HosListBand3M = {};
SetSharedVariable[HosListBand3M];

ParallelDo[
  HamCurr[k_] := Ham1tn1[k[[1]] - k[[2]], k[[1]] + k[[2]], k[[3]], Delt];

 $\theta_{\text{Curr}} = 8.46;$ 
CurrResIn =  $10^{-3}$ ;
HOSFound = False;
NoTry = 1;

While[NoTry ≤ 4 && HOSFound == False,
  TaylorPoly =
    Chop[TaylorExpandBand[HamCurr(*The Hamiltonian*), {0,  $\pi$  // N,  $\theta_{\text{Curr}}$ }
      (*the (k,t) point at which we are going to series expand.*), 3
      (*Band to series expand*), 2(*Degree of Taylor polynomial*),

```

```

"Dimension" → 2(*k-space dimension*), "TuningDegree" → 2
(*Degree of tuning parameter terms*),
"TuningSymbol" → "δθ"(*Symbols for the tuning parameters*),
"Resolution" → 10-4(*Resolution below which we shall kill terms*),
"SampleDirection" → {0.333, 0.779, 0.1335}
(*A sample k-vector that will be used for diagonalising symbolic
matrices. This is not needed in principle since we will
generate a random one in the routine if this is not provided*),
"Messages" → False(*YesMessage*)], 10-6];

HesDet = (D[TaylorPoly[[1, 3]], {p1, 2}] × D[TaylorPoly[[1, 3]], {p2, 2}] -
(D[TaylorPoly[[1, 3]], p1, p2])2) /. {p1 → 0, p2 → 0} // Simplify;

If[Chop[ReplaceAll[HesDet, {δθ → 0}]] == 0,
  HOSFound = True;
];

δθSolns = Solve[HesDet == 0, δθ, Reals];

MinSoln = 1;
Do[
  If[Abs[ReplaceAll[δθ, δθSolns[[l]]]] < Abs[ReplaceAll[δθ, δθSolns[[MinSoln]]]],
    MinSoln = l;
  ],
  {l, 1, Length[δθSolns]};

θCurr = θCurr + δθ /. δθSolns[[MinSoln]];
];

If[HOSFound == True,
  TaylorPoly =
  Chop[TaylorExpandBand[HamCurr(*The Hamiltonian*), {0, π // N, θCurr}
    (*the (k,t) point at which we are going to series expand.*), 3
    (*Band to series expand*), 4(*Degree of Taylor polynomial*),
    "Dimension" → 2(*k-space dimension*), "TuningDegree" → 0
    (*Degree of tuning parameter terms*),
    "TuningSymbol" → "δθ"(*Symbols for the tuning parameters*),
    "Resolution" → 10-4(*Resolution below which we shall kill terms*),
    "SampleDirection" → {0.333, 0.779, 0.1335}
    (*A sample k-vector that will be used for diagonalising symbolic
matrices. This is not needed in principle since we will
generate a random one in the routine if this is not provided*),
    "Messages" → False(*YesMessage*)], 10-6];

AppendTo[HosListBand3M, {Delt, θCurr, NoTry, Total[
  Chop[ReplaceAll[TaylorPoly[[1]], {p1 → kx, p2 → ky, δθ → 0}]], CurrResln]]];

```

```
,
Print[Style["No HOS found in the range!", Red]];
];

, {Delt, 0.001, 0.008, 0.001}]
```

We will have to sort the list since it was constructed using a parallelized Do loop:

```
In[320]:= HosListBand3M = SortBy[HosListBand3M, First];
```

Using this, we can diagnose the HOS and view the θ_{crit} and Taylor expansion for each Δ :

```
In[332]:= Do[
Print[" $\Delta_{\text{stag}}$  = ", Round[1000 hosdata[[1]]],
"meV. Search converged after ", hosdata[[3]], " iterations."];
Print["\t" <> " $\theta_{\text{crit}}$  = ", NumberForm[hosdata[[2]], {4, 2}],
", Tayl = ", NumberForm[hosdata[[4]], {4, 3}]];
DiagnoseHOS[Chop[hosdata[[4]], 10-2]];
Print[
"*****"]

, {hosdata, HosListBand3M}]
```

$\Delta_{\text{stag}} = 1\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.082 - 2.296 k_x^4 + 0.103 k_x^3 k_y + 4.190 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 2.296 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 2\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.083 - 1.255 k_x^4 + 0.103 k_x^3 k_y + 2.109 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 1.255 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 3\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.084 - 0.908 k_x^4 + 0.103 k_x^3 k_y + 1.415 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 0.908 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 4\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.085 - 0.735 k_x^4 + 0.103 k_x^3 k_y + 1.069 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 0.735 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 5\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.086 - 0.631 k_x^4 + 0.103 k_x^3 k_y + 0.860 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 0.631 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 6\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.087 - 0.562 k_x^4 + 0.103 k_x^3 k_y + 0.722 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 0.562 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 7\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.088 - 0.512 k_x^4 + 0.103 k_x^3 k_y + 0.623 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 0.512 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 8\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.089 - 0.475 k_x^4 + 0.103 k_x^3 k_y + 0.548 k_x^2 k_y^2 - 0.103 k_x k_y^3 - 0.475 k_y^4$$

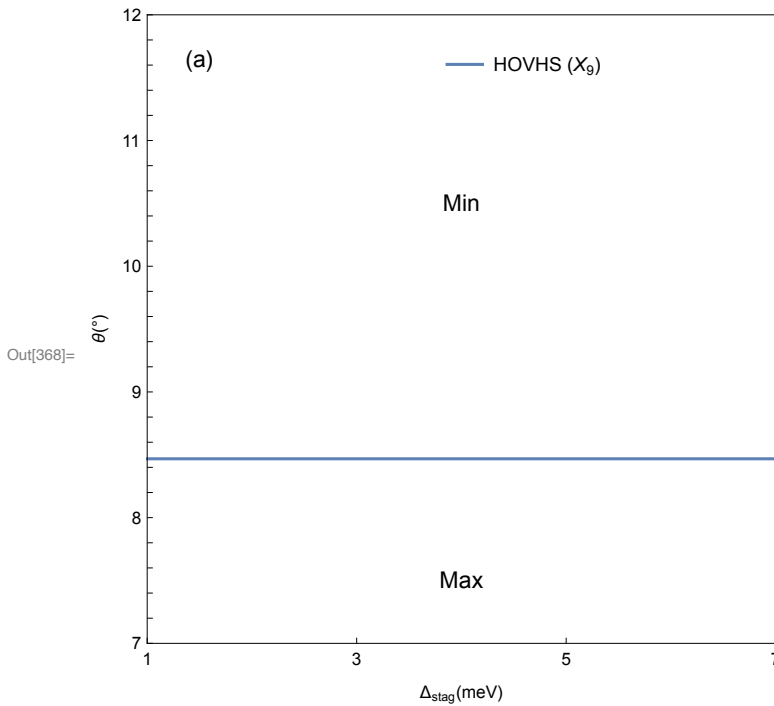
Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

```

In[367]:= FitFunc3M = Interpolation[HosListBand3M[All, 1 ;; 2]];
Panel1 = Show[(*PlotBand9,*)Plot[FitFunc3M[x / 1000],
  {x, 1, 7}, FrameLabel → {" $\Delta_{\text{stag}}$  (meV)", " $\theta$  (°)"}, PlotLegends → Placed[
    {Style["HOVHS ( $X_9$ )", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
  PlotRange → {{1, 7}, {7, 12}}, Frame → True, AspectRatio → 1,
  FrameTicks → {{Automatic, None}, {{1, 3, 5, 7}, None}}],
Graphics[Text[Style["Max", FontFamily → "Arial", FontSize → 12], {4, 7.5}]],
Graphics[Text[Style["Min", FontFamily → "Arial", FontSize → 12], {4, 10.5}]],
Graphics[Text[Style["(a)", FontFamily → "Arial", FontSize → 12], {1.5, 11.65}]]]

```



Band 4

```

In[340]:= HosListBand4M = {};
SetSharedVariable[HosListBand4M];

ParallelDo[
  HamCurr[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]], k[[3]], Delt];

   $\theta_{\text{Curr}} = 8.46$ ;
  CurrResIn =  $10^{-3}$ ;
  HOSFound = False;
  NoTry = 1;

  While[NoTry ≤ 4 && HOSFound == False,
    TaylorPoly =
      Chop[TaylorExpandBand[HamCurr(*The Hamiltonian*), {0,  $\pi$  // N,  $\theta_{\text{Curr}}$ }
        (*the (k,t) point at which we are going to series expand.*), 4
        (*Band to series expand*), 2(*Degree of Taylor polynomial*),

```

```

"Dimension" → 2(*k-space dimension*), "TuningDegree" → 2
(*Degree of tuning parameter terms*),
"TuningSymbol" → "δθ"(*Symbols for the tuning parameters*),
"Resolution" → 10-4(*Resolution below which we shall kill terms*),
"SampleDirection" → {0.333, 0.779, 0.1335}
(*A sample k-vector that will be used for diagonalising symbolic
matrices. This is not needed in principle since we will
generate a random one in the routine if this is not provided*),
"Messages" → False(*YesMessage*)], 10-6];

HesDet = (D[TaylorPoly[[1, 3]], {p1, 2}] × D[TaylorPoly[[1, 3]], {p2, 2}] -
(D[TaylorPoly[[1, 3]], p1, p2])2) /. {p1 → 0, p2 → 0} // Simplify;

If[Chop[ReplaceAll[HesDet, {δθ → 0}]] == 0,
  HOSFound = True;
];

δθSolns = Solve[HesDet == 0, δθ, Reals];

MinSoln = 1;
Do[
  If[Abs[ReplaceAll[δθ, δθSolns[[l]]]] < Abs[ReplaceAll[δθ, δθSolns[[MinSoln]]]],
    MinSoln = l;
  ],
  {l, 1, Length[δθSolns]}];

θCurr = θCurr + δθ /. δθSolns[[MinSoln]];
];

If[HOSFound == True,
  TaylorPoly =
  Chop[TaylorExpandBand[HamCurr(*The Hamiltonian*), {0, π // N, θCurr}
    (*the (k,t) point at which we are going to series expand.*), 4
    (*Band to series expand*), 4(*Degree of Taylor polynomial*),
    "Dimension" → 2(*k-space dimension*), "TuningDegree" → 0
    (*Degree of tuning parameter terms*),
    "TuningSymbol" → "δθ"(*Symbols for the tuning parameters*),
    "Resolution" → 10-4(*Resolution below which we shall kill terms*),
    "SampleDirection" → {0.333, 0.779, 0.1335}
    (*A sample k-vector that will be used for diagonalising symbolic
    matrices. This is not needed in principle since we will
    generate a random one in the routine if this is not provided*),
    "Messages" → False(*YesMessage*)], 10-6];

AppendTo[HosListBand4M, {Delt, θCurr, NoTry, Total[
  Chop[ReplaceAll[TaylorPoly[[1]], {p1 → kx, p2 → ky, δθ → 0}]], CurrResln]]];

```

```
,
Print[Style["No HOS found in the range!", Red]];
];

, {Delt, 0.001, 0.008, 0.001}]
```

We will have to sort the list since it was constructed using a parallelized Do loop:

```
In[343]:= HosListBand4M = SortBy[HosListBand4M, First];
```

Using this, we can diagnose the HOS and view the θ_{crit} and Taylor expansion for each Δ :

```
In[344]:= Do[
Print[" $\Delta_{\text{stag}}$  = ", Round[1000 hosdata[[1]]],
"meV. Search converged after ", hosdata[[3]], " iterations."];
Print["\t" <> " $\theta_{\text{crit}}$  = ", NumberForm[hosdata[[2]], {4, 2}],
", Tayl = ", NumberForm[hosdata[[4]], {4, 3}]];
DiagnoseHOS[Chop[hosdata[[4]], 10-2]];
Print[
"*****"]

, {hosdata, HosListBand4M}]
```

$\Delta_{\text{stag}} = 1\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.080 + 1.866 k_x^4 - 0.103 k_x^3 k_y - 4.133 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 1.866 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 2\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.079 + 0.826 k_x^4 - 0.103 k_x^3 k_y - 2.053 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.826 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 3\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.078 + 0.479 k_x^4 - 0.103 k_x^3 k_y - 1.359 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.479 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:
Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 4\text{meV}$. Search converged after 1 iterations.

$$\theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.077 + 0.305 k_x^4 - 0.103 k_x^3 k_y - 1.012 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.305 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 5\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.076 + 0.201 k_x^4 - 0.103 k_x^3 k_y - 0.804 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.201 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 6\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.075 + 0.132 k_x^4 - 0.103 k_x^3 k_y - 0.665 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.132 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 7\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.074 + 0.082 k_x^4 - 0.103 k_x^3 k_y - 0.566 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.082 k_y^4$$

Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

$\Delta_{\text{stag}} = 8\text{meV}$. Search converged after 1 iterations.

$$\Theta_{\text{crit}} = 8.47, \text{ Tayl} = -0.073 + 0.045 k_x^4 - 0.103 k_x^3 k_y - 0.492 k_x^2 k_y^2 + 0.103 k_x k_y^3 + 0.045 k_y^4$$

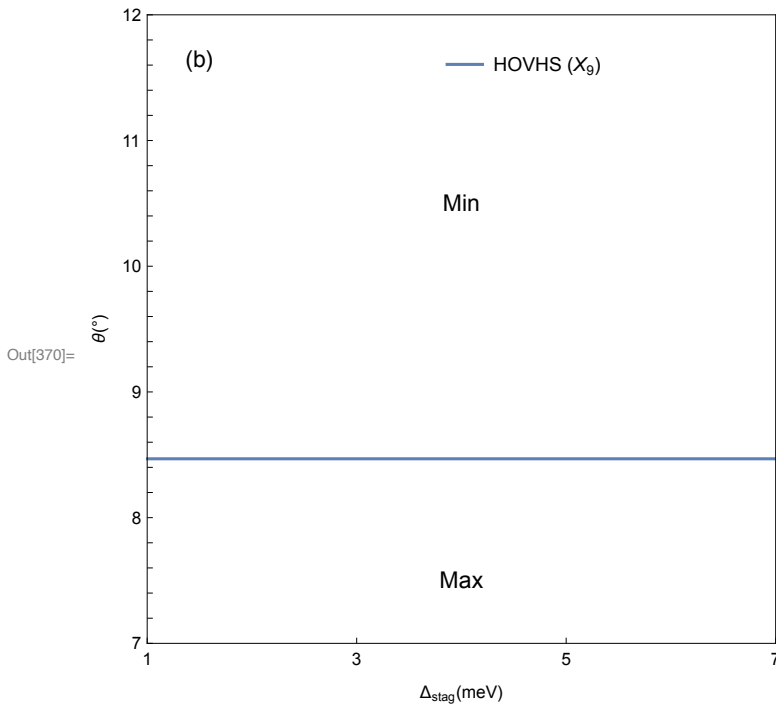
Polynomial has corank 2. It is 5-determinate. Its determinacy is either 5 or 4
and its codimension is 8. Comparing with the known list of singularities:

Polynomial has a catastrophe belonging to the X_9 singularity class.

```

In[369]:= FitFunc4M = Interpolation[HosListBand4M[All, 1 ;; 2]];
Panel2 = Show[(*PlotBand9,*)Plot[FitFunc4M[x / 1000],
  {x, 1, 7}, FrameLabel → {" $\Delta_{\text{stag}}$  (meV)", " $\theta$  (°)"}, PlotLegends → Placed[
    {Style["HOVHS ( $X_9$ )", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
  PlotRange → {{1, 7}, {7, 12}}, Frame → True, AspectRatio → 1,
  FrameTicks → {{Automatic, None}, {{1, 3, 5, 7}, None}}],
  Graphics[Text[Style["Max", FontFamily → "Arial", FontSize → 12], {4, 7.5}]],
  Graphics[Text[Style["Min", FontFamily → "Arial", FontSize → 12], {4, 10.5}]],
  Graphics[Text[Style["(b)", FontFamily → "Arial", FontSize → 12], {1.5, 11.65}]]]

```



Phase Diagram

```

In[855]:=  $\theta_{\text{min}} = 7;$ 
 $\theta_{\text{max}} = 12 (*9.6*);$ 

cm = 72 / 2.54;

TicsFontSize = 6;
AxesFontSize = 8;
RegionFontColour = LightGray;
FigLength = 3.5 cm;
LeftPadding = 0.5 cm;
RightPadding = 0.2 cm;
BottomPadding = 0.5 cm;
TopPadding = 0.15 cm;
xTicsLabeled = {{7, "7"}, {8, "8"}, {9, "9"}, {10, "10"}, {11, "11"}, {12, "12"}};
xTics = {7, 8, 9, 10, 11, 12};

```

```
yTics = {1, 3, 5, 7};
```

```
VHsColour = { $\frac{(*125*)161}{255}$ ,  $\frac{(*9*)93}{255}$ ,  $\frac{(*184*)216}{255}$ , 1(*0.65*)};
MinColour = { $\frac{(*9*)59}{255}$ ,  $\frac{(*73*)96}{255}$ ,  $\frac{(*184*)196}{255}$ , 1(*0.65*)};
MaxColour = { $\frac{(*207*)242}{255}$ ,  $\frac{(*17*)70}{255}$ ,  $\frac{(*51*)70}{255}$ , 1(*0.65*)};
```

```
PanA = ParametricPlot[
  {{v FitFunc4M[u / 1000] +  $\theta_{\min}$  (1 - v), u}, {(1 - v) FitFunc4M[u / 1000] +  $\theta_{\max}$  v, u}},
  {u, 1, 7}, {v, 0, 1}, PlotRange → {{ $\theta_{\min}$ ,  $\theta_{\max}$ }, {1, 7}}, Frame → True,
  PlotStyle → {RGBColor[MaxColour], RGBColor[MinColour]}, AspectRatio → 1,
  (*FrameTicks→{True,True},*)(*FrameLabel→{None,Style[" $\Delta_{\text{nem}}$  (%)",
    FontFamily→"Arial",FontSize→AxesFontSize,FontColor→Black]},*)
  FrameTicksStyle → {{Directive[Black, FontFamily → "Arial", TicsFontSize],
    Directive[Black, FontOpacity → 0, FontSize → 0]},
    {Directive[Black, FontOpacity → 0, FontSize → 0],
    Directive[Black, FontOpacity → 0, FontSize → 0]}},
  FrameTicks → {{yTics, yTics}, {xTics, xTics}},
  ImagePadding → {{LeftPadding, RightPadding}, {0.6 TopPadding, TopPadding}},
  ImageSize → FigLength];
```

```
PanAp2 =
  ParametricPlot[{FitFunc4M[u / 1000], u}, {u, 1, 7}, Axes → False, Frame → False,
  PlotStyle → {Black, Thickness[0.018]}, PlotRange → {{ $\theta_{\min}$ ,  $\theta_{\max}$ }, {1, 7}},
  PlotLegends → Placed[LineLegend[{Style["X9", FontFamily → "Arial",
    FontSize → TicsFontSize, FontColor → RegionFontColour]},
    LegendMarkerSize → {10, 1.3}], {{0.75, 0.92}, {0.5, 0.5}}];
```

```
FullTopPan = Labeled[
  Show[PanA, PanAp2, Graphics[Rotate[Text[Style["Maximum", FontFamily → "Arial",
    FontColor → RegionFontColour, FontSize → TicsFontSize], {7.75, 4}],
    90 Degree]], Graphics[Text[Style["Minimum", FontFamily → "Arial",
    FontColor → RegionFontColour, FontSize → TicsFontSize], {10.5, 4}]]],
  {Style[" $\Delta_{\text{st}}$  (meV)", FontFamily → "Arial", FontSize → AxesFontSize,
    FontColor → Black], ""},
  {Left, Bottom}, Spacings → {0, 0}, RotateLabel → True]
```

```
PanB = ParametricPlot[
  {{v FitFunc3M[u / 1000] +  $\theta_{\min}$  (1 - v), u}, {(1 - v) FitFunc3M[u / 1000] +  $\theta_{\max}$  v, u}},
  {u, 1, 7}, {v, 0, 1}, PlotRange → {{ $\theta_{\min}$ ,  $\theta_{\max}$ }, {1, 7}}, Frame → True,
  PlotStyle → {RGBColor[MaxColour], RGBColor[MinColour]}, AspectRatio → 1,
  FrameTicksStyle → {{Directive[Black, FontFamily → "Arial", TicsFontSize],
    Directive[Black, FontOpacity → 0, FontSize → 0]},
    {Directive[Black, FontFamily → "Arial", TicsFontSize],
```

```

Directive[Black, FontOpacity → 0, FontSize → 0]]},
FrameTicks → {{yTics, yTics}, {xTicsLabeled, xTics}},
ImagePadding → {{LeftPadding, RightPadding}, {BottomPadding, 0.6 TopPadding}},
ImageSize → FigLength];

```

```

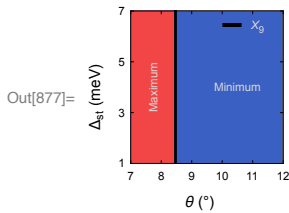
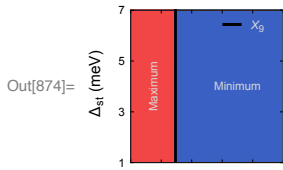
PanBp2 = ParametricPlot[{FitFunc3M[u / 1000], u}, {u, 1, 7},
  Axes → False, Frame → False, PlotStyle → {Black, Thickness[0.018]},
  PlotLegends → Placed[LineLegend[{Style["X9", FontFamily → "Arial",
    FontSize → TicsFontSize, FontColor → RegionFontColour]},
    LegendMarkerSize → {10, 1.3}], {{0.75, 0.92}, {0.5, 0.5}}]];

```

```

FullBottomPan = Labeled[
  Show[PanB, PanBp2, Graphics[Rotate[Text[Style["Maximum", FontFamily → "Arial",
    FontColor → RegionFontColour, FontSize → TicsFontSize], {7.75, 4}],
    90 Degree]], Graphics[Text[Style["Minimum", FontFamily → "Arial",
    FontColor → RegionFontColour, FontSize → TicsFontSize], {10.5, 4}]]],
  {Style["Δst (meV)", FontFamily → "Arial", FontSize → AxesFontSize,
    FontColor → Black], Style["θ (°)", FontFamily → "Arial",
    FontSize → AxesFontSize, FontColor → Black]},
  {Left, Bottom}, Spacings → {0, 0}, RotateLabel → True]

```

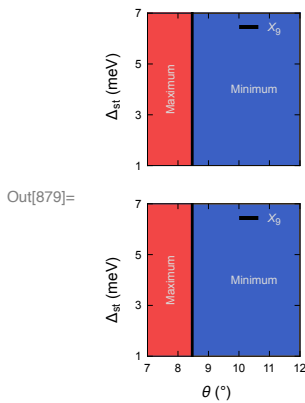


These can be labeled and assembled together into final form suitable for publications

```

In[879]:= GraphicsGrid[{{FullTopPan}, {FullBottomPan}}, Spacings → {0, -8}]

```



We will generate the band structure for $\theta = 6^\circ$, θ_{crit} and $\theta = 10^\circ$.


```
In[ ]:= Ham1[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]], 6, 0.005]
```

```
Bnds1 = GenerateBandStructure[Ham1,  
  HSymmPts, "OrbitalProjection" → False, "TotalPoints" → 200];
```

```
In[732]:= plt1 = PlotBandStructure[Bnds1, (*{-0.042,0.012}*){-0.2, 0.1}, AspectRatio → 2,  
  "yLabel" → {(*Label*)"E (eV)", (*Font Size*)AxesFontSize, (*Font Color*)  
    Black, (*Font Family*)"Arial"}, "xLabel" → {AxesFontSize, Black, "Arial"},  
  "yTicks" → {TicsFontSize, Black, "Helvetica"}, "LineThickness" → 0.009,  
  "LineColorScheme" → {LightRed}, (*Dividing Lines*)"DividingLines" →  
    {(*Dashing[.])*0.01, (*Color*)Gray, (*Thickness*)0.004},  
  "PlotKeyLegend" → {{Style["θ = 6°", FontSize → TicsFontSize]}, {0.25, 0.95}}];
```

```
In[ ]:= Ham2[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]], θcrit, 0.005]
```

```
Bnds2 = GenerateBandStructure[Ham2,  
  HSymmPts, "OrbitalProjection" → False, "TotalPoints" → 400];
```

```
In[733]:= plt2 = PlotBandStructure[Bnds2, (*{-0.042,0.012}*){-0.2, 0.1}, AspectRatio → 2,  
  "yLabel" → {(*Label*)"E (eV)", (*Font Size*)AxesFontSize, (*Font Color*)  
    Black, (*Font Family*)"Arial"}, "xLabel" → {AxesFontSize, Black, "Arial"},  
  "yTicks" → {TicsFontSize, Black, "Helvetica"}, "LineThickness" → 0.009,  
  "LineColorScheme" → {Brown}, (*Dividing Lines*)  
  "DividingLines" → {(*Dashing[.])*0.01, (*Color*)  
    Gray, (*Thickness*)0.004}, "PlotKeyLegend" →  
    {{Style["θ = 8.47°", FontSize → TicsFontSize]}, {0.25, 0.9}}];
```

```
In[ ]:= Ham3[k_] := Hamltn1[k[[1]] - k[[2]], k[[1]] + k[[2]], 10, 0.005]
```

```
Bnds3 = GenerateBandStructure[HamOther2,  
  HSymmPts, "OrbitalProjection" → False, "TotalPoints" → 200];
```

```
In[738]:= plt3 = PlotBandStructure[Bnds3, (*{-0.042,0.012}*){-0.2, 0.1}, AspectRatio → 2,  
  "yLabel" → {(*Label*)"E (eV)", (*Font Size*)AxesFontSize, (*Font Color*)  
    Black, (*Font Family*)"Arial"}, "xLabel" → {AxesFontSize, Black, "Arial"},  
  "yTicks" → {TicsFontSize, Black, "Helvetica"}, "LineThickness" → 0.009,  
  "LineColorScheme" → {LightBlue}, (*Dividing Lines*)  
  "DividingLines" → {(*Dashing[.])*0.01, (*Color*)  
    Gray, (*Thickness*)0.004}, "PlotKeyLegend" →  
    {{Style["θ = 10°", FontSize → TicsFontSize]}, {0.25, 0.85}}];
```

```
In[880]:= BandsFinal = Show[plt1, plt3, plt2, ImageSize → 4.5 cm]
```

