Tuning the SOC gap and M point higher order Van Hove singularities in the surface bands of $Sr_2 RuO_4$

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Loading the Library

We first load the library by executing the following:

```
In[99]:= AppendTo[$Path, StringDelete[NotebookDirectory[], "/Sr2RuO4"] <> "Package"];
<< BandUtilities`
```

Outline of the strategy

We will begin by loading and interpolating the tight-binding models for various values of θ and then separately load and interpolate through the models with nematic term added. We will then interpolate linearly between the nematicity free model and the model with the nematic term to generate a continuously tunable model.

Interpolating between the Wannier90 files

Ingredients needed for symmetrization

In[3]:=
```
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 pepole'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[11]:= FileLocn = NotebookDirectory[] <> "unrenormalized2/";

W90Data = LoadInterpolateTBMs[{FileLocn <> "Sr2RuO4_0deg.dat",
    FileLocn <> "Sr2RuO4_1deg.dat", FileLocn <> "Sr2RuO4_2deg.dat",
    FileLocn <> "Sr2RuO4_3deg.dat", FileLocn <> "Sr2RuO4_4deg.dat",
    FileLocn <> "Sr2RuO4_5deg.dat", FileLocn <> "Sr2RuO4_6deg.dat",
    FileLocn <> "Sr2RuO4_7deg.dat", FileLocn <> "Sr2RuO4_8deg.dat",
    FileLocn <> "Sr2RuO4_9deg.dat", FileLocn <> "Sr2RuO4_10deg.dat",
    FileLocn <> "Sr2RuO4_11deg.dat", FileLocn <> "Sr2RuO4_12deg.dat"},
   {0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12}, "Symmetries" → SymmetryList,
   "OrbitalCentres" → AtomLocations, "ParameterSymbol" → "θ"];

Hamltn1[k1_, k2_, θ_] = W90Data〚1〛;
```

```
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
```

Phenomenological spin orbit term

We now construct the phenomenological SOC terms:

In[14]:=
```
Lx = {{0, 0, i}, {0, 0, 0}, {-i, 0, 0}};
Ly = {{0, 0, 0}, {0, 0, i}, {0, -i, 0}};
Lz = {{0, -i, 0}, {i, 0, 0}, {0, 0, 0}};

Hupup = 1/2 Lz;
Hupdown = 1/2 (Lx + i Ly);
Hdownup = 1/2 (Lx - i Ly);
Hdowndown = -1/2 Lz;
Zero2 = ConstantArray[0, {3, 3}];


HSOC = Join[Join[Hupup, Zero2, Hupdown, Zero2, 2],
   Join[Zero2, Hupup, Zero2, Hupdown, 2], Join[Hdownup, Zero2,
    Hdowndown, Zero2, 2], Join[Zero2, Hdownup, Zero2, Hdowndown, 2]];
```

Reconstructing the full interpolated Hamiltonian

The full Hamiltonian incorporating SOC with tunable SOC strength and tunable θ. A version for the $\sqrt{2} \times \sqrt{2}$ unit cell that is tailor made for fitting to the ARPES data is also defined (since the bulk has one Ru atom per unit cell, its Brillouin zone has twice the area of the default surface band BZ, which is also 'rotated' by 45°).

In[23]:=
```
Hamiltonian1[k1_, k2_, θ_, λ_] =
  0.5 (ArrayFlatten[IdentityMatrix[2]⊗Hamltn1[k1, k2, θ]] +
     λ HSOC + ComplexExpand[ConjugateTranspose[
       ArrayFlatten[IdentityMatrix[2]⊗Hamltn1[k1, k2, θ]] + λ HSOC]]);
```

We can check the eigenvalues at a high symmetry point to see if the symmetrisation was successful, and has eliminated the weak splitting of degeneracies at the high symmetry points

Loading and interpolating the nematic models

In[27]:=
```
FileLocn2 = NotebookDirectory[] <> "renormalized/";

W90Data2 = LoadInterpolateTBMs[
   {FileLocn2 <> "Sr2RuO4_EXP_Monolayer_1theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_1theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_2theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_3theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_4theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_5theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_6theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_7theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_8theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_9theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_10theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <> "Sr2RuO4_EXP_Monolayer_11theta_0phi1_0phi2_hr_sym_soc_nem.dat",
    FileLocn2 <>
     "Sr2RuO4_EXP_Monolayer_12theta_0phi1_0phi2_hr_sym_soc_nem.dat"},
   {0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12}, "ParameterSymbol" → "θ"];

Hamiltonian2[k1_, k2_, θ_] = W90Data2[[1]];
```

```
Invalid or no lattice vectors provided! Using unit vectors.

Tight-binding data files loaded.

Space dimension: 3

Number of orbitals: 12

Number of supercells: 49

Number of models/data-files to interpolate: 13

Number of lines in the data files:
 {1723, 1723, 1723, 1723, 1707, 1723, 1723, 1723, 1723, 1723, 1723, 1723, 1723}

Interpolating between the Hamiltonians.

No valid symmetrization scheme
  provided! We will not symmetrize the loaded Hamiltonian.
```

Comparing the nematic and symmetric models

For the sake of plotting, let us define the Hamiltonians evaluated at $\theta = 8°$ with and without the nematic term

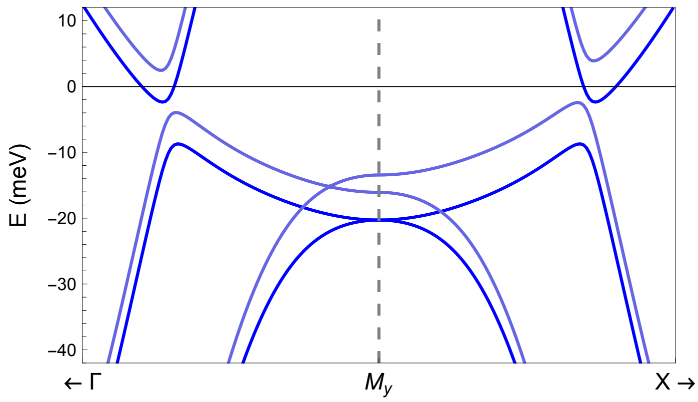
In[33]:=
```
HamTemp[k_] := 1000 × 0.2444 Hamiltonian1[k[[1]] - k[[2]], k[[1]] + k[[2]], 8, 0.175]
HamTempNem[k_] := 1000 Hamiltonian2[k[[1]] - k[[2]], k[[1]] + k[[2]], 8]
```

Using these the bands can be generated

In[74]:=
```
HSymmPts =
  {{{0, π - 3.869 × 0.36}, "← Γ"}, {{0, π}, "My"}, {{3.869 × 0.36, π}, "X →"}};
Bnd1 = GenerateBandStructure[HamTemp, HSymmPts];
Bnd2 = GenerateBandStructure[HamTempNem, HSymmPts];
```

In[77]:=
```
plt1 = PlotBandStructure[Bnd1, {-42, 12},
   "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
     12, (*Font Color*)Black, (*Font Family*)"Arial"},
   "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
   "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[0, 0, 1]}];

plt2 = PlotBandStructure[Bnd2, {-42, 12},
   "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
     12, (*Font Color*)Black, (*Font Family*)"Arial"},
   "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
   "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[0.4, 0.4, 0.9]}];

Show[plt1, plt2]
```

Out[79]=



The degeneracy at the M_y point has been lifted which is to be expected since the nematic term breaks the r_{xy} reflection symmetry that causes the degeneracy.

A continuously θ(°) and Δ_{nem}(%) tuned model

```
HamiltonianNemTunedmeV[k1_, k2_, θ_, Δ_] =
  (1 - Δ) 1000 × 0.2444 Hamiltonian1[k1 - k2, k1 + k2, θ, 0.175] +
   1000 Δ Hamiltonian2[k1 - k2, k1 + k2, θ];

HamltnTuned[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, k⟦3⟧, k⟦4⟧]

HamTempNem2[k_] :=
 HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, 8, 2(*Nematicity set to 2%*)]
```

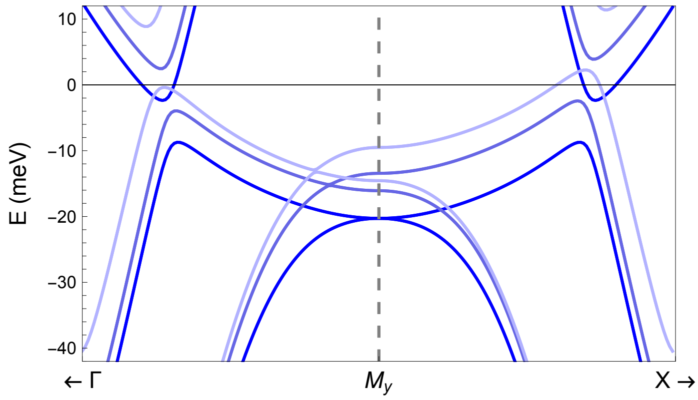
Checking the interpolation

In[80]:=
```
Bnd3 = GenerateBandStructure[HamTempNem2, HSymmPts];
```

In[81]:=
```
plt3 = PlotBandStructure[Bnd3, {-42, 12},
   "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
     12, (*Font Color*)Black, (*Font Family*)"Arial"},
   "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
   "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[0.7, 0.7, 1]}];
```

```
Show[plt1, plt2, plt3]
```

Out[82]=



We can see that the interpolation scheme has worked.

Iterating through Δ_{nem} and hunting for HOS

Let us outline the strategy that we shall adopt below. We iterate through a few values of Δ_{nem} including 0%, 1% and 2%. At each Δ_{nem}, we will try to tune the M point singularity and the SOC gap critical points to a HOS. We note down the θ_{crit} and the series expansion of the four bands.

Now the bands(points) of interest are 5&6(M point), 7&8(M point), 7&8(SOC gap) and 9&10(SOC gap). For 5&6(M point) and 7&8(M point), tuning to HOS is simpler. We are already at a critical point, namely the high symmetry M point. We compute det(Hes) as a function of $\delta\theta$ and set it to zero to solve for $\delta\theta$. If we repeat this a few times we get θ_{crit}. But for the SOC gap critical points, we have to adopt a different strategy since the location of the critical point is not fixed and changes with θ and Δ_{nem}.

We will use a two-pronged strategy: first we choose a range of θ to investigate, say 8° to 10°. We locate the $\boldsymbol{k}_{VHS}$ for the angles at the end points of the range and compute the Hessian determinant. If they are of opposite sign, we expect the Hessian determinant to vanish somewhere in between. We will then use binary search to locate this θ_{crit}. We have to do this separately for both the bands, and on either sides of the SOC gap (which have been made inequivalent by the nematic term).

Firstly, we have to identify the range of $\boldsymbol{k}$ in which the SOC critical points seem to exist by plotting the dispersion for Δ_{nem} = 0%, 1%, 2% and 4% and $\theta = 7°, 8°, ..., 11°$. This is needed since we need to identify a suitable range for the LocateCriticalPoint routine to work to find the actual $\boldsymbol{k}_{VHS}$.

Evolution of the band-structure

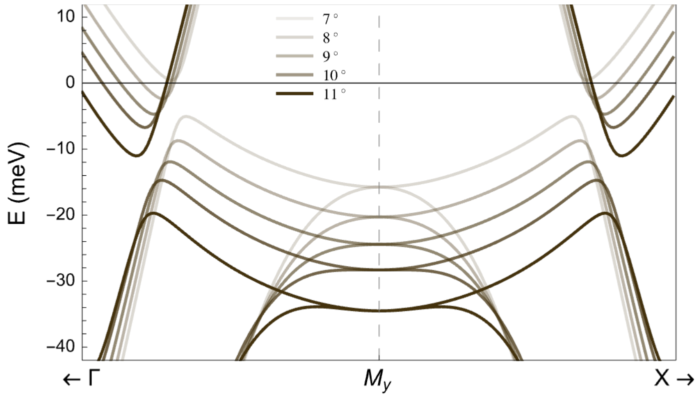
We plot a spaghetti plot showing the evolution of the band-structure with θ for different choices of Δ_{nem} (0%, 1% and 2%).

```
HSymmPtsNoLabel =
  {{{0, π - 3.869 × 0.35}, ""}, {{0, π}, ""}, {{3.869 × 0.35, π}, ""}};
AngleList = {7, 8, 9, 10, 11};

OpacityList = {0.1, 0.2, 0.35, 0.5, 1};
ColourChoice = {67/255, 49/255, 12/255}(*{45/255, 38/255, 87/255}*);
(*This for one choice of colour scheme -
 with a fixed colour and varying transparency given by the alpha channel.*)
```

1) $\Delta_{nem} = 0 \times \%$

```
In[83]:= BandDataList1 = First@Last@Reap[Do[
        HamCurr[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], angle, 0.];

        Sow[GenerateBandStructure[HamCurr, HSymmPts]];
        , {angle, AngleList}]];

In[84]:= BandPlotList1 = First@Last@Reap[Do[
        Sow[PlotBandStructure[BandDataList1[[i]], {-42, 12}(*meV range*),
           "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
             12, (*Font Color*)Black, (*Font Family*)"Arial"},
           "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
           "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[ColourChoice[[1]],
              ColourChoice[[2]], ColourChoice[[3]], OpacityList[[i]]]},
           "PlotKeyLegend" → {Style[ToString[AngleList[[i]]] °, FontSize → 8,
              FontFamily → "Times"], Scaled[{0.31, 1.01 - i / 19.}]}]];
        , {i, 1, Length[AngleList]}]];
```

In[85]:=
```
SpaghettiPlot1 = Show[BandPlotList1]
```

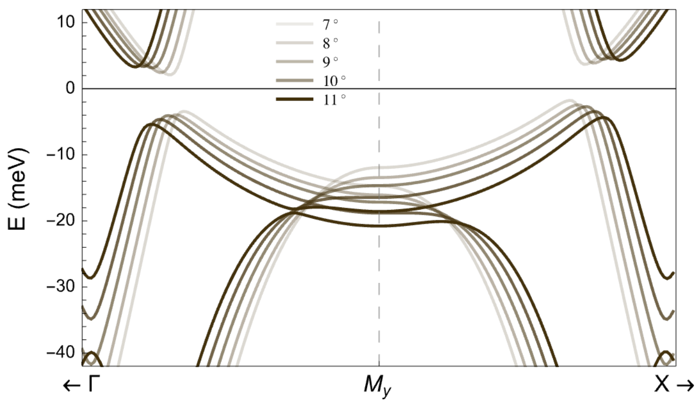
Out[85]=


2) Δ_{nem} = 1 × %

In[86]:=
```
BandDataList2 = First@Last@Reap[Do[
        HamCurr[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, angle, 1.];

        Sow[GenerateBandStructure[HamCurr, HSymmPts]];
        , {angle, AngleList}]];
```

In[87]:=
```
BandPlotList2 = First@Last@Reap[Do[
        Sow[PlotBandStructure[BandDataList2⟦i⟧, {-42, 12}(*meV range*),
            "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
              12, (*Font Color*)Black, (*Font Family*)"Arial"},
            "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
            "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[ColourChoice⟦1⟧,
               ColourChoice⟦2⟧, ColourChoice⟦3⟧, OpacityList⟦i⟧]},
            "PlotKeyLegend" → {Style[ToString[AngleList⟦i⟧] °, FontSize → 8,
               FontFamily → "Times"], Scaled[{0.31, 1.01 - i / 19.}]}]];
        , {i, 1, Length[AngleList]}]];
```

In[88]:=
```
SpaghettiPlot2 = Show[BandPlotList2]
```

Out[88]=


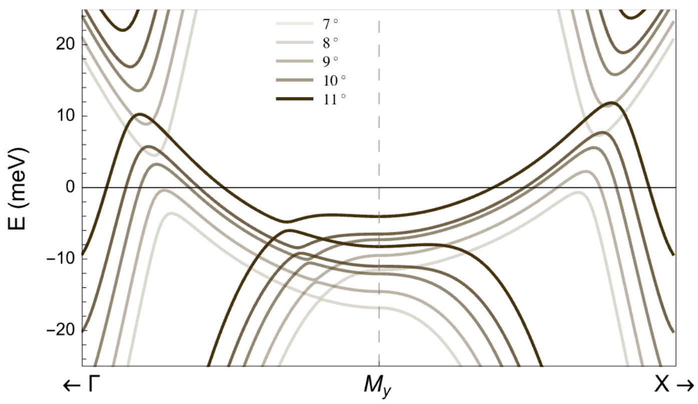
3) $\Delta_{nem} = 2 \times \%$

In[89]:=
```
BandDataList3 = First@Last@Reap[Do[
    HamCurr[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, angle, 2.];

    Sow[GenerateBandStructure[HamCurr, HSymmPts]];
    , {angle, AngleList}]];
```

In[90]:=
```
BandPlotList3 = First@Last@Reap[Do[
    Sow[PlotBandStructure[BandDataList3⟦i⟧, {-25, 25}(*meV range*),
      "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
        12, (*Font Color*)Black, (*Font Family*)"Arial"},
      "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
      "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[ColourChoice⟦1⟧,
         ColourChoice⟦2⟧, ColourChoice⟦3⟧, OpacityList⟦i⟧]},
      "PlotKeyLegend" → {Style[ToString[AngleList⟦i⟧] °, FontSize → 8,
         FontFamily → "Times"], Scaled[{0.31, 1.01 - i / 19.}]}]];
    , {i, 1, Length[AngleList]}]];
```

In[92]:=
```
SpaghettiPlot3 = Show[BandPlotList3]
```

Out[92]=



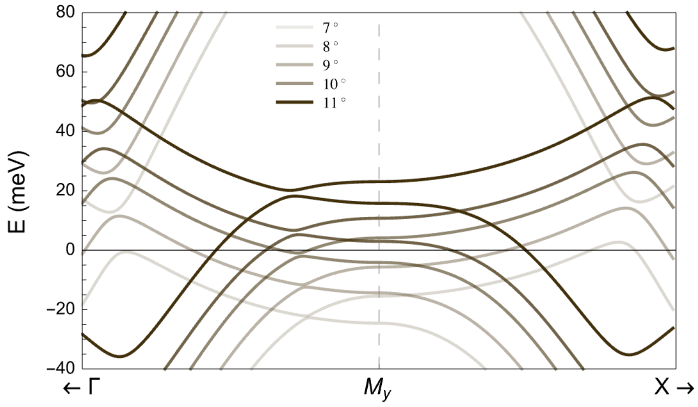
3) $\Delta_{nem} = 4 \times \%$

In[93]:=
```
BandDataList4 = First@Last@Reap[Do[
    HamCurr[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, angle, 4.];

    Sow[GenerateBandStructure[HamCurr, HSymmPts]];
    , {angle, AngleList}]];
```

In[94]:=
```
BandPlotList4 = First@Last@Reap[Do[
    Sow[PlotBandStructure[BandDataList4[[i]], {-40, 80}(*meV range*),
      "AspectRatio" → 3/5, "yLabel" → {(*Label*)"E (meV)", (*Font Size*)
        12, (*Font Color*)Black, (*Font Family*)"Arial"},
      "xLabel" → {12, Black, "Arial"}, "yTicks" → {9, Black, "Arial"},
      "LineThickness" → 0.005, "LineColorScheme" → {RGBColor[ColourChoice[[1]],
         ColourChoice[[2]], ColourChoice[[3]], OpacityList[[i]]]},
      "PlotKeyLegend" → {Style[ToString[AngleList[[i]]] °, FontSize → 8,
         FontFamily → "Times"], Scaled[{0.31, 1.01 - i / 19.}]}]];
    , {i, 1, Length[AngleList]}]];
```

In[95]:=
```
SpaghettiPlot4 = Show[BandPlotList4]
```

Out[95]=



Evolution of the nature of the critical points in the SOC gap

In this section, we look at the evolution of the nature of the critical points as we change Δ_{nem} and θ, that is whether they are maxima, minima or saddles.

Upper VHS - Band 9, part 1

In[119]:=
```
Do[
  Print["Δnem=", Delt, "%:"];

  Do[

   HamCurr[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θCurr, Delt];

   kVHSTrialLow = {0.6 × 3.869 × 0.36, π // N};
   kVHSTrialUp = {3.869 × 0.36, π // N};

   (*Finding true kVHS:*)
   {kVHS, CritPtFound} = LocateCriticalPoint[
     HamCurr, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
     "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

   If[CritPtFound == True,
    TaylorPoly =
     Chop[Total[TaylorExpandBand[HamCurr, kVHS, 9, 2, "Messages" → False][[1]]] /.
       {p1 → kx, p2 → ky}, 10^-2];

    Print["\t", "θ = ", θCurr, ", kcrit = ", kVHS, ", Tayl = ", TaylorPoly];
    ,
    Print["Critical point could not be found for θ = ", θCurr];
   ]

   , {θCurr, 8, 11, 1}];

 , {Delt, 0, 4, 1(*0.25*)}];
```

Δ_{nem}=0%:

θ = 8, k_{crit} = {1.01581, 3.14159}, Tayl = $-2.36331 + 529.026\,k_x^2 - 9.47938\,k_y^2$

θ = 9, k_{crit} = {1.05733, 3.14159}, Tayl = $-4.71827 + 503.4\,k_x^2 + 4.02982\,k_y^2$

θ = 10, k_{crit} = {1.09814, 3.14159}, Tayl = $-6.73067 + 483.824\,k_x^2 + 16.2413\,k_y^2$

θ = 11, k_{crit} = {1.13796, 3.14159}, Tayl = $-11.0382 + 472.719\,k_x^2 + 26.8556\,k_y^2$

Δ_{nem}=1%:

θ = 8, k_{crit} = {1.00831, 3.14159}, Tayl = $3.88659 + 508.026\,k_x^2 - 10.0838\,k_y^2$

θ = 9, k_{crit} = {1.05033, 3.14159}, Tayl = $4.459 + 485.567\,k_x^2 + 3.53534\,k_y^2$

θ = 10, k_{crit} = {1.09162, 3.14159}, Tayl = $4.5194 + 467.958\,k_x^2 + 15.8555\,k_y^2$

θ = 11, k_{crit} = {1.13192, 3.14159}, Tayl = $4.30303 + 458.082\,k_x^2 + 26.5837\,k_y^2$

Δ_{nem}=2%:

θ = 8, k_{crit} = {1.06639, 3.14159}, Tayl = $11.3763 + 416.234\,k_x^2 - 13.2742\,k_y^2$

θ = 9, k_{crit} = {1.10587, 3.14159}, Tayl = $15.7941 + 403.497\,k_x^2 - 0.812546\,k_y^2$

θ = 10, k_{crit} = {1.1442, 3.14159}, Tayl = $18.8672 + 398.826\,k_x^2 + 10.2062\,k_y^2$

θ = 11, k_{crit} = {1.18092, 3.14159}, Tayl = $23.7056 + 404.734\,k_x^2 + 19.483\,k_y^2$

Δ_{nem}=3%:

θ = 8, k_{crit} = {1.15559, 3.14159}, Tayl = $19.6969 + 388.477\,k_x^2 - 17.618\,k_y^2$

θ = 9, k_{crit} = {1.19051, 3.14159}, Tayl = $28.3895 + 383.784\,k_x^2 - 7.04354\,k_y^2$

θ = 10, k_{crit} = {1.22406, 3.14159}, Tayl = $34.8767 + 388.926\,k_x^2 + 2.14796\,k_y^2$

θ = 11, k_{crit} = {1.25604, 3.14159}, Tayl = $45.1184 + 405.141\,k_x^2 + 9.79735\,k_y^2$

Δ_{nem}=4%:

θ = 8, k_{crit} = {1.25345, 3.14159}, Tayl = $29.0708 + 404.815\,k_x^2 - 21.4064\,k_y^2$

θ = 9, k_{crit} = {1.28423, 3.14159}, Tayl = $42.0426 + 404.599\,k_x^2 - 12.7704\,k_y^2$

θ = 10, k_{crit} = {1.31408, 3.14159}, Tayl = $51.9031 + 413.994\,k_x^2 - 5.23332\,k_y^2$

θ = 11, k_{crit} = {1.34329, 3.14159}, Tayl = $67.4569 + 432.759\,k_x^2 + 1.15399\,k_y^2$

We see that all the HOS points indeed likely lie in the range [8°,11°] since the coefficient of k_y^2 changes sign for all the values of Δ_{nem} in this range. Also, **the critical point changes from an ordinary saddle to an ordinary minimum** as we increase θ at each Δ_{nem}. Now for band 8 (downward dispersing):

Lower VHS - Band 8, part 1

In[118]:=
```
Do[
  Print["Δnem=", Delt, "%:"];

  Do[

   HamCurr[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, θCurr, Delt];

   kVHSTrialLow = {0.5 × 3.869 × 0.35, π // N};
   kVHSTrialUp = {0.9 × 3.869 × 0.35, π // N};

   (*Finding true kVHS:*)
   {kVHS, CritPtFound} = LocateCriticalPoint[
     HamCurr, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
     "SanityChecks" → False, "MaxIterations" → 28, "Resolution" → 10^-2];

   If[CritPtFound == True,
    TaylorPoly =
     Chop[Total[TaylorExpandBand[HamCurr, kVHS, 8, 2, "Messages" → False]⟦1⟧] /.
       {p1 → kx, p2 → ky}, 10^-2];

    Print["\t", "θ = ", θCurr, ", kcrit = ", kVHS, ", Tayl = ", TaylorPoly];
    ,
    Print["Critical point could not be found for θ = ", θCurr];
   ]

   , {θCurr, 8, 11, 1}];

 , {Delt, 0, 3, 1(*0.25*)}];
```

Δ_{nem}=0%:

θ = 8, k_{crit} = {0.943277, 3.14159}, Tayl = $-8.71343 - 417.359\, k_x^2 - 12.3465\, k_y^2$

θ = 9, k_{crit} = {0.981329, 3.14159}, Tayl = $-11.9083 - 400.277\, k_x^2 + 1.12069\, k_y^2$

θ = 10, k_{crit} = {1.02021, 3.14159}, Tayl = $-14.7072 - 388.262\, k_x^2 + 13.1978\, k_y^2$

θ = 11, k_{crit} = {1.06041, 3.14159}, Tayl = $-19.695 - 382.709\, k_x^2 + 23.3541\, k_y^2$

Δ_{nem}=1%:

θ = 8, k_{crit} = {0.933392, 3.14159}, Tayl = $-2.42802 - 395.894\, k_x^2 - 12.9932\, k_y^2$

θ = 9, k_{crit} = {0.971956, 3.14159}, Tayl = $-2.69943 - 381.479\, k_x^2 + 0.585187\, k_y^2$

θ = 10, k_{crit} = {1.01135, 3.14159}, Tayl = $-3.43275 - 371.822\, k_x^2 + 12.7885\, k_y^2$

θ = 11, k_{crit} = {1.05201, 3.14159}, Tayl = $-4.34178 - 367.689\, k_x^2 + 23.0969\, k_y^2$

Δ_{nem}=2%:

θ = 8, k_{crit} = {0.970287, 3.14159}, Tayl = $2.26882 - 310.083\, k_x^2 - 16.7735\, k_y^2$

θ = 9, k_{crit} = {1.00791, 3.14159}, Tayl = $5.59709 - 304.037\, k_x^2 - 4.49169\, k_y^2$

θ = 10, k_{crit} = {1.04781, 3.14159}, Tayl = $7.72889 - 304.834\, k_x^2 + 6.01401\, k_y^2$

θ = 11, k_{crit} = {1.09056, 3.14159}, Tayl = $11.8771 - 313.623\, k_x^2 + 13.9943\, k_y^2$

Δ_{nem}=3%:

θ = 8, k_{crit} = {1.05042, 3.14159}, Tayl = $7.27525 - 293.395\, k_x^2 - 20.7362\, k_y^2$

θ = 9, k_{crit} = {1.08798, 3.14159}, Tayl = $14.7984 - 292.943\, k_x^2 - 10.7027\, k_y^2$

θ = 10, k_{crit} = {1.12924, 3.14159}, Tayl = $20.4623 - 301.146\, k_x^2 - 2.82157\, k_y^2$

θ = 11, k_{crit} = {1.17407, 3.14159}, Tayl = $30.366 - 318.71\, k_x^2 + 2.28758\, k_y^2$

Here too we see that for all the Δ_{nem} the HOS likely lies in the range [8°,11°]. Also, we see that **the critical point changes from an ordinary maximum to an ordinary saddle** as we increase θ at each Δ_{nem} up to 3%.

Using binary search to find HOVHs in the SOC gap

Band 9, part 1

In[207]:=
```
NoIterns = 5;
CurrResln = 10^-2;
kVHSTrialLow = {0.6 × 3.869 × 0.36, π // N};
kVHSTrialUp = {3.869 × 0.36, π // N};

HosListBand9 = {};
SetSharedVariable[HosListBand9];

ParallelDo[
 HamCurr[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, k⟦3⟧, Delt];
```

```
NoTry = 0;
HOSFound = False;
HOSPossible = True;
θmax = 10;
θmin = 8;

(*Print["Binary search initiated for Δnem = ",Delt];*)

While[NoTry ≤ 14 && HOSFound == False && HOSPossible == True,
 HamCurrUp[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmax, Delt];
 HamCurrDown[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmin, Delt];

 (*We compute the Hessian determinant for θmax*)
 (*Finding true kVHS:*)
 {kVHSmax, CritPtFound} = LocateCriticalPoint[
   HamCurrUp, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

 TaylorPolyMax = TaylorExpandBand[HamCurrUp, kVHSmax, 9, 2, "Messages" → False];

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMax = Chop[TaylorPolyMax, CurrResln];

 (*Print["kcrit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

 (*We now compute the Hessian determinant for θmin*)
 (*Finding true kVHS:*)
 {kVHSmin, CritPtFound} = LocateCriticalPoint[
   HamCurrDown, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

 TaylorPolyMin =
  TaylorExpandBand[HamCurrDown, kVHSmin, 9, 2, "Messages" → False];

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMin = Chop[TaylorPolyMin, CurrResln];
```

```
(*Print["k_crit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

(*Now we begin the binary search if the
 Hessian determinants computed above are opposite in sign*)
If[Sign[HesDetMax] == -Sign[HesDetMin] && HOSFound == False && HOSPossible == True,

 θmid = 0.5 (θmax + θmin);
 HamCurrMid[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmid, Delt];

 (*Finding true kVHS1:*)
 {kVHSmid, CritPtFound} = LocateCriticalPoint[
   HamCurrMid, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

 TaylorPolyMid =
  TaylorExpandBand[HamCurrMid, kVHSmid, 9, 2, "Messages" → False];

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMid = Chop[TaylorPolyMid, CurrResln];

 (*Print["k_crit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMid = Chop[TaylorPolyMid, CurrResln];

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

 If[Chop[HesDet, 1.] == 0,
  HOSFound = True;
  ,
  If[Sign[HesDet] == Sign[HesDetMax],
   θmax = θmid;
   ,
```

```
      If[Sign[HesDet] == Sign[HesDetMin],
       θmin = θmid;
      ]
     ]
    ];

    NoTry++;
    ,
    If[HOSFound == False,
     Print[Style["No HOS in the range!", Red]];
     HOSPossible = False;
    ]
   ];
  ];

  If[HOSFound == True,
   Print["Δnem = ", Delt,
    ". Binary search converged after ", NoTry, " iterations."];
   Print["θcrit=", θmid, ", det[Hes]=", HesDet,
    ", Tayl = ", Chop[Total[TaylorPolyMid[[1]]] /. {p1 → kx, p2 → ky}]];
   AppendTo[HosListBand9, {Delt, θmid}];
   ,
   Print[Style["No HOS in the range!", Red]];
  ];
  , {Delt, 0, 3, 0.25}]
```

(kernel 6) Δ_{nem} = 1.. Binary search converged after 7 iterations.

(kernel 6) θ_{crit}=8.73438, det[Hes]=0., Tayl = $4.23394 + 491.382\, k_x^2$

(kernel 1) Δ_{nem} = 3.. Binary search converged after 8 iterations.

(kernel 1) θ_{crit}=9.74219, det[Hes]=0., Tayl = $33.8245 + 386.602\, k_x^2$

(kernel 8) Δ_{nem} = 0.. Binary search converged after 8 iterations.

(kernel 8) θ_{crit}=8.69531, det[Hes]=0., Tayl = $-4.0873 + 511.035\, k_x^2$

(kernel 7) Δ_{nem} = 0.5. Binary search converged after 8 iterations.

(kernel 7) θ_{crit}=8.67969, det[Hes]=0., Tayl = $-0.224357 + 524.967\, k_x^2$

(kernel 3) Δ_{nem} = 2.5. Binary search converged after 10 iterations.

(kernel 3) θ_{crit}=9.35742, det[Hes]=0., Tayl = $24.2157 + 385.642\, k_x^2$

(kernel 4) Δ_{nem} = 2.. Binary search converged after 10 iterations.

(kernel 4) θ_{crit}=9.06836, det[Hes]=0., Tayl = $16.1091 + 402.723\, k_x^2$

(kernel 2) Δ_{nem} = 2.75. Binary search converged after 10 iterations.

(kernel 2) θ_{crit}=9.53711, det[Hes]=0., Tayl = $28.8717 + 384.118\, k_x^2$

(kernel 5) Δ_{nem} = 1.5. Binary search converged after 11 iterations.

(kernel 5) θ_{crit}=8.8623, det[Hes]=0., Tayl = $9.56419 + 440.202\, k_x^2$

(kernel 6) Δ_{nem} = 1.25. Binary search converged after 8 iterations.

(kernel 6) θ_{crit}=8.78906, det[Hes]=0., Tayl = 6.77168 + 465.273 k_x^2

(kernel 8) Δ_{nem} = 0.25. Binary search converged after 11 iterations.

(kernel 8) θ_{crit}=8.67871, det[Hes]=0., Tayl = -2.2114 + 523.537 k_x^2

(kernel 4) Δ_{nem} = 2.25. Binary search converged after 10 iterations.

(kernel 4) θ_{crit}=9.20117, det[Hes]=0., Tayl = 19.9499 + 391.846 k_x^2

(kernel 7) Δ_{nem} = 0.75. Binary search converged after 11 iterations.

(kernel 7) θ_{crit}=8.69824, det[Hes]=0., Tayl = 1.91293 + 513.132 k_x^2

(kernel 5) Δ_{nem} = 1.75. Binary search converged after 10 iterations.

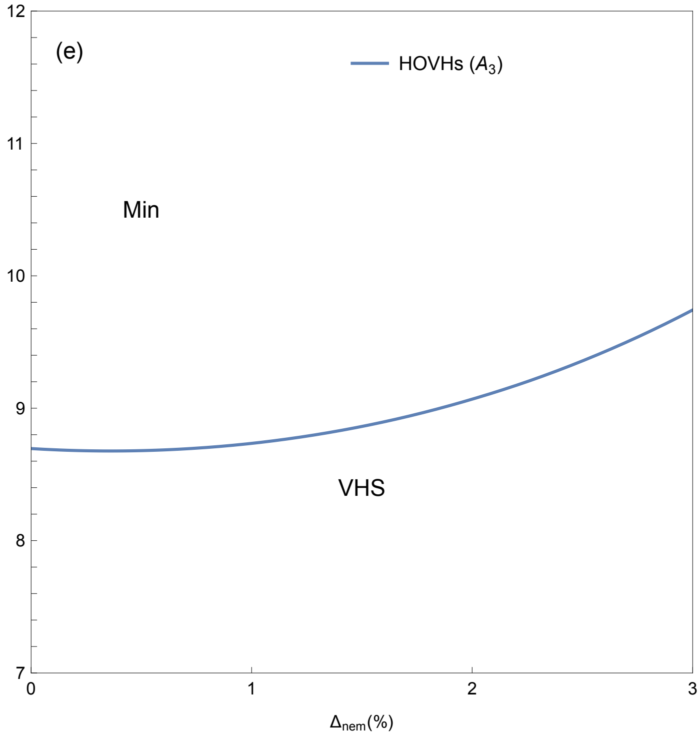
(kernel 5) θ_{crit}=8.95508, det[Hes]=0., Tayl = 12.6591 + 418.975 k_x^2

In[142]:=
```
HosListBand9 = SortBy[HosListBand9, First]
```

Out[142]=
```
{{0., 8.69531}, {0.25, 8.67871}, {0.5, 8.67969}, {0.75, 8.69824},
 {1., 8.73438}, {1.25, 8.78906}, {1.5, 8.8623}, {1.75, 8.95508}, {2., 9.06836},
 {2.25, 9.20117}, {2.5, 9.35742}, {2.75, 9.53711}, {3., 9.74219}}
```

In[637]:=
```
FitFunc1 = Interpolation[HosListBand9];
PlotBand9 = ListPlot[HosListBand9];
PanelE = Show[(*PlotBand9,*)Plot[FitFunc1[x], {x, 0, 3},
    FrameLabel → {"Δnem(%)", (*"θ(°)"*)None}, PlotLegends → Placed[
      {Style["HOVHs (A3)", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
    PlotRange → {{0, 3}, {7, 12}}, Frame → True, AspectRatio → 1,
    FrameTicks → {{Automatic, None}, {{0, 1, 2, 3}, None}}],
  Graphics[Text[Style["VHS", FontFamily → "Arial", FontSize → 12], {1.5, 8.4}]],
  Graphics[Text[Style["Min", FontFamily → "Arial", FontSize → 12], {0.5, 10.5}]],
  Graphics[
    Text[Style["(e)", FontFamily → "Arial", FontSize → 12], {0.175, 11.7}]]]
```

Out[639]=



Band 8, part 1

In[196]:=
```
NoIterns = 5;
CurrResln = 10^-2;
kVHSTrialLow = {0.5 × 3.869 × 0.35, π // N};
kVHSTrialUp = {0.9 × 3.869 × 0.35, π // N};

HosListBand8 = {};
SetSharedVariable[HosListBand8];

ParallelDo[
 HamCurr[k_] := HamiltonianNemTunedmeV[k〚1〛, k〚2〛, k〚3〛, Delt];

 NoTry = 0;
 HOSFound = False;
 HOSPossible = True;
 θmax = 11;
 θmin = 8;

 (*Print["Binary search initiated for Δnem = ",Delt];*)

 While[NoTry ≤ 18 && HOSFound == False && HOSPossible == True,
  HamCurrUp[k_] := HamiltonianNemTunedmeV[k〚1〛, k〚2〛, θmax, Delt];
  HamCurrDown[k_] := HamiltonianNemTunedmeV[k〚1〛, k〚2〛, θmin, Delt];

  (*We compute the Hessian determinant for θmax*)
  (*Finding true kVHS:*)
  {kVHSmax, CritPtFound} = LocateCriticalPoint[
    HamCurrUp, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
    "SanityChecks" → True, "MaxIterations" → 28, "Resolution" → 10^-2];

  TaylorPolyMax = TaylorExpandBand[HamCurrUp, kVHSmax, 8, 2, "Messages" → False];
  TaylorPolyMax = Chop[TaylorPolyMax, CurrResln];

  (*Print["kcrit,max = ",kVHSmax,TaylorPolyMax〚1〛];*)

  HesDetMax = (D[TaylorPolyMax〚1, 3〛, {p1, 2}] × D[TaylorPolyMax〚1, 3〛, {p2, 2}] -
       (D[TaylorPolyMax〚1, 3〛, p1, p2])^2) /. {p1 → 0, p2 → 0} // Simplify;

  If[CritPtFound == False,
   HOSPossible = False;
   (*Print["Critical point not found for θmax at Δnem = ",Delt,"."];*)
  ];
```

```
(*We now compute the Hessian determinant for θmin*)
(*Finding true kVHS:*)
{kVHSmin, CritPtFound} = LocateCriticalPoint[
  HamCurrDown, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
  "SanityChecks" → True, "MaxIterations" → 28, "Resolution" → 10^-2];

TaylorPolyMin =
 TaylorExpandBand[HamCurrDown, kVHSmin, 8, 2, "Messages" → False];
TaylorPolyMin = Chop[TaylorPolyMin, CurrResln];

(*Print["k_crit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

If[CritPtFound == False,
 HOSPossible = False;
 (*Print["Critical point not found for θmin at Δnem = ",Delt,"."];*)
];

(*Now we begin the binary search if the
 Hessian determinants computed above are opposite in sign*)
If[Sign[HesDetMax] == -Sign[HesDetMin] && HOSFound == False && HOSPossible == True,

 θmid = 0.5 (θmax + θmin);
 HamCurrMid[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmid, Delt];

 (*Finding true kVHS1:*)
 {kVHSmid, CritPtFound} = LocateCriticalPoint[
   HamCurrMid, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 28, "Resolution" → 10^-2];

 TaylorPolyMid =
  TaylorExpandBand[HamCurrMid, kVHSmid, 8, 2, "Messages" → False];
 TaylorPolyMid = Chop[TaylorPolyMid, CurrResln];

 (*Print["k_crit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

 If[CritPtFound == False,
  HOSPossible = False;
  (*Print["Critical point not found for θmid at Δnem = ",Delt,"."];*)
 ];
```

```
      If[Chop[HesDetMid, 1.] == 0,
       HOSFound = True;
       ,
       If[Sign[HesDetMid] == Sign[HesDetMax],
        θmax = θmid;
        ,
        If[Sign[HesDetMid] == Sign[HesDetMin],
         θmin = θmid;
        ]
       ]
      ];

      NoTry++;
      ,
      If[HOSFound == False,
       Print[Style["No HOS in the range!", Red]];
       HOSPossible = False;
      ]
     ];
    ];

    If[HOSFound == True,
     Print["Δnem = ", Delt,
      ". Binary search converged after ", NoTry, " iterations."];
     Print["θcrit=", θmid, ", det[Hes]=", HesDetMid,
      ", Tayl = ", Chop[Total[TaylorPolyMid[[1]]] /. {p1 → kx, p2 → ky}]];
     AppendTo[HosListBand8, {Delt, θmid}];
     ,
     Print[Style["No HOS in the range!", Red]];
    ];
    , {Delt, 0, 3, 0.25}]
```

(kernel 8) Δ_{nem} = 0.. Binary search converged after 7 iterations.

(kernel 8) θ_{crit}=8.91406, det[Hes]=0., Tayl = $-11.6625 - 401.535\, k_x^2$

(kernel 1) Δ_{nem} = 3.. Binary search converged after 8 iterations.

(kernel 1) θ_{crit}=10.5664, det[Hes]=-0.000106631, Tayl = $22.8522 - 310.467\, k_x^2 - 0.0103262\, k_x\, k_y$

(kernel 4) Δ_{nem} = 2.. Binary search converged after 8 iterations.

(kernel 4) θ_{crit}=9.39453, det[Hes]=0., Tayl = $6.87135 - 302.988\, k_x^2$

(kernel 6) Δ_{nem} = 1.. Binary search converged after 9 iterations.

(kernel 6) θ_{crit}=8.95508, det[Hes]=0., Tayl = $-2.69961 - 382.237\, k_x^2$

(kernel 7) Δ_{nem} = 0.5. Binary search converged after 9 iterations.

(kernel 7) θ_{crit}=8.88477, det[Hes]=0., Tayl = $-6.94277 - 414.511\, k_x^2$

(kernel 2) Δ_{nem} = 2.75. Binary search converged after 10 iterations.

(kernel 2) θ_{crit}=10.1064, det[Hes]=0., Tayl = 17.2836 − 298.616 k_x^2

(kernel 3) $\triangle_{nem}$ = 2.5. Binary search converged after 10 iterations.

(kernel 3) θ_{crit}=9.80176, det[Hes]=0., Tayl = 13.4432 − 294.303 k_x^2

(kernel 5) $\triangle_{nem}$ = 1.5. Binary search converged after 11 iterations.

(kernel 5) θ_{crit}=9.12646, det[Hes]=0., Tayl = 1.66114 − 334.565 k_x^2

(kernel 4) $\triangle_{nem}$ = 2.25. Binary search converged after 9 iterations.

(kernel 4) θ_{crit}=9.57617, det[Hes]=0., Tayl = 9.97966 − 295.728 k_x^2

(kernel 8) $\triangle_{nem}$ = 0.25. Binary search converged after 11 iterations.

(kernel 8) θ_{crit}=8.88623, det[Hes]=0., Tayl = −9.21966 − 413.253 k_x^2

(kernel 6) $\triangle_{nem}$ = 1.25. Binary search converged after 10 iterations.

(kernel 6) θ_{crit}=9.02832, det[Hes]=0., Tayl = −0.581924 − 357.603 k_x^2

(kernel 7) $\triangle_{nem}$ = 0.75. Binary search converged after 11 iterations.

(kernel 7) θ_{crit}=8.90674, det[Hes]=0., Tayl = −4.78992 − 402.981 k_x^2

(kernel 5) $\triangle_{nem}$ = 1.75. Binary search converged after 9 iterations.

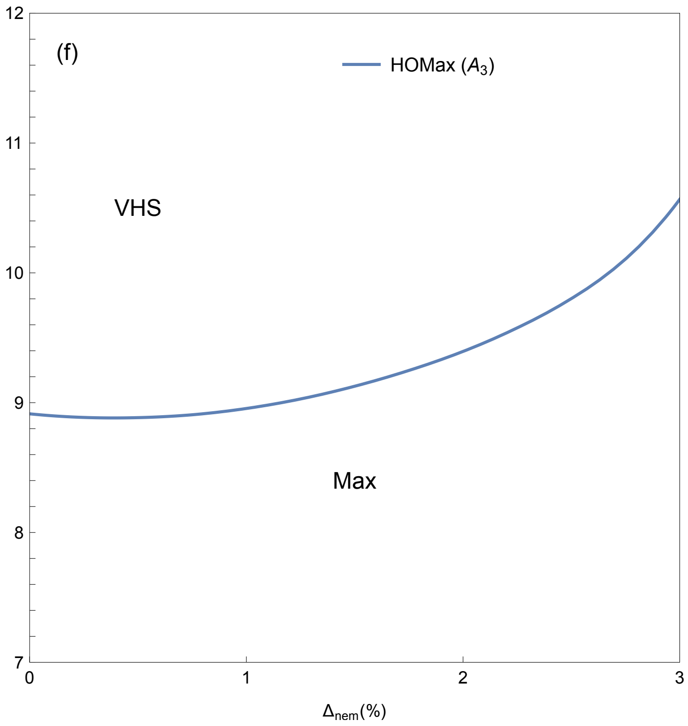
(kernel 5) θ_{crit}=9.24805, det[Hes]=0., Tayl = 4.12031 − 315.973 k_x^2

In[203]:= **HosListBand8 = SortBy[HosListBand8, First]**

Out[203]= {{0., 8.91406}, {0.25, 8.88623}, {0.5, 8.88477}, {0.75, 8.90674}, {1., 8.95508}, {1.25, 9.02832}, {1.5, 9.12646}, {1.75, 9.24805}, {2., 9.39453}, {2.25, 9.57617}, {2.5, 9.80176}, {2.75, 10.1064}, {3., 10.5664}}

In[640]:=
```
FitFunc2 = Interpolation[HosListBand8];
PlotBand8 = ListPlot[HosListBand8];
PanelF = Show[(*PlotBand9,*)Plot[FitFunc2[x], {x, 0, 3},
   FrameLabel → {"Δnem(%)", (*"θ(°)"*)None}, PlotLegends → Placed[
     {Style["HOMax (A3)", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
   PlotRange → {{0, 3}, {7, 12}}, Frame → True, AspectRatio → 1,
   FrameTicks → {{Automatic, None}, {{0, 1, 2, 3}, None}}],
  Graphics[Text[Style["Max", FontFamily → "Arial", FontSize → 12], {1.5, 8.4}]],
  Graphics[Text[Style["VHS", FontFamily → "Arial", FontSize → 12], {0.5, 10.5}]],
  Graphics[
   Text[Style["(f)", FontFamily → "Arial", FontSize → 12], {0.175, 11.7}]]]
```

Out[642]=



Band 9, part 2

In[217]:=
```
NoIterns = 5;
CurrResln = 10^-2;
kVHSTrialLow = {0, π - 3.869 × 0.36};
kVHSTrialUp = {0, π - 0.6 × 3.869 × 0.36};

HosListBand9p2 = {};
SetSharedVariable[HosListBand9p2];

ParallelDo[
 HamCurr[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], k[[3]], Delt];

 NoTry = 0;
 HOSFound = False;
 HOSPossible = True;
```

```
θmax = 10;
θmin = 8;

(*Print["Binary search initiated for Δnem = ",Delt];*)

While[NoTry ≤ 14 && HOSFound == False && HOSPossible == True,
 HamCurrUp[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmax, Delt];
 HamCurrDown[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmin, Delt];

 (*We compute the Hessian determinant for θmax*)
 (*Finding true kVHS:*)
 {kVHSmax, CritPtFound} = LocateCriticalPoint[
   HamCurrUp, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

 TaylorPolyMax = TaylorExpandBand[HamCurrUp, kVHSmax, 9, 2, "Messages" → False];

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMax = Chop[TaylorPolyMax, CurrResln];

 (*Print["kcrit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

 (*We now compute the Hessian determinant for θmin*)
 (*Finding true kVHS:*)
 {kVHSmin, CritPtFound} = LocateCriticalPoint[
   HamCurrDown, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

 TaylorPolyMin =
  TaylorExpandBand[HamCurrDown, kVHSmin, 9, 2, "Messages" → False];

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMin = Chop[TaylorPolyMin, CurrResln];

 (*Print["kcrit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

 HesDetMin = (D[TaylorPolyMin[[1, 3]], {p1, 2}] × D[TaylorPolyMin[[1, 3]], {p2, 2}] -
```

```
    (D[TaylorPolyMin⟦1, 3⟧, p1, p2])^2) /. {p1 → 0, p2 → 0} // Simplify;

(*Now we begin the binary search if the
 Hessian determinants computed above are opposite in sign*)
If[Sign[HesDetMax] == -Sign[HesDetMin] && HOSFound == False && HOSPossible == True,

 θmid = 0.5 (θmax + θmin);
 HamCurrMid[k_] := HamiltonianNemTunedmeV[k⟦1⟧, k⟦2⟧, θmid, Delt];

 (*Finding true kVHS1:*)
 {kVHSmid, CritPtFound} = LocateCriticalPoint[
   HamCurrMid, kVHSTrialLow, kVHSTrialUp, 9, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 24, "Resolution" → 10^-2];

 TaylorPolyMid =
  TaylorExpandBand[HamCurrMid, kVHSmid, 9, 2, "Messages" → False];

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMid = Chop[TaylorPolyMid, CurrResln];

 (*Print["k_crit,max = ",kVHSmax,TaylorPolyMax⟦1⟧];*)

 HesDetMid = (D[TaylorPolyMid⟦1, 3⟧, {p1, 2}] × D[TaylorPolyMid⟦1, 3⟧, {p2, 2}] -
      (D[TaylorPolyMid⟦1, 3⟧, p1, p2])^2) /. {p1 → 0, p2 → 0} // Simplify;

 If[CritPtFound == False,
  HOSPossible = False;
 ];

 TaylorPolyMid = Chop[TaylorPolyMid, CurrResln];

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

 If[Chop[HesDet, 1.] == 0,
  HOSFound = True;
  ,
  If[Sign[HesDet] == Sign[HesDetMax],
   θmax = θmid;
   ,
   If[Sign[HesDet] == Sign[HesDetMin],
    θmin = θmid;
   ]
```

```
    ]
   ];

   NoTry++;
   ,
   If[HOSFound == False,
    Print[Style["No HOS in the range!", Red]];
    HOSPossible = False;
   ]
  ];
 ];

 If[HOSFound == True,
  Print["Δnem = ", Delt,
   ". Binary search converged after ", NoTry, " iterations."];
  Print["θcrit=", θmid, ", det[Hes]=", HesDet,
   ", Tayl = ", Chop[Total[TaylorPolyMid[[1]]] /. {p1 → kx, p2 → ky}]];
  AppendTo[HosListBand9p2, {Delt, θmid}];
  ,
  Print[Style["No HOS in the range!", Red]];
 ];
 , {Delt, 0, 3, 0.25}]
```

(kernel 6) Δ_{nem} = 1.. Binary search converged after 6 iterations.

(kernel 6) θ_{crit}=8.65625, det[Hes]=0., Tayl = $2.82964 + 531.172\, k_y^2$

(kernel 7) Δ_{nem} = 0.5. Binary search converged after 7 iterations.

(kernel 7) θ_{crit}=8.64063, det[Hes]=0., Tayl = $-0.87683 + 546.402\, k_y^2$

(kernel 3) Δ_{nem} = 2.5. Binary search converged after 8 iterations.

(kernel 3) θ_{crit}=9.17969, det[Hes]=0., Tayl = $20.6695 + 448.428\, k_y^2$

(kernel 8) Δ_{nem} = 0.. Binary search converged after 8 iterations.

(kernel 8) θ_{crit}=8.69531, det[Hes]=0., Tayl = $-4.0873 + 511.035\, k_y^2$

(kernel 1) Δ_{nem} = 3.. Binary search converged after 8 iterations.

(kernel 1) θ_{crit}=9.53906, det[Hes]=0., Tayl = $30.1774 + 455.236\, k_y^2$

(kernel 2) Δ_{nem} = 2.75. Binary search converged after 9 iterations.

(kernel 2) θ_{crit}=9.34766, det[Hes]=0., Tayl = $25.2007 + 449.627\, k_y^2$

(kernel 4) Δ_{nem} = 2.. Binary search converged after 10 iterations.

(kernel 4) θ_{crit}=8.91992, det[Hes]=0., Tayl = $13.1493 + 460.175\, k_y^2$

(kernel 5) Δ_{nem} = 1.5. Binary search converged after 11 iterations.

(kernel 5) θ_{crit}=8.74707, det[Hes]=0., Tayl = $7.36585 + 491.107\, k_y^2$

(kernel 6) Δ_{nem} = 1.25. Binary search converged after 9 iterations.

(kernel 6) θ_{crit}=8.69141, det[Hes]=0., Tayl = $4.97067 + 511.489\, k_y^2$

(kernel 7) Δ_{nem} = 0.75. Binary search converged after 10 iterations.

(kernel 7) θ_{crit}=8.63867, det[Hes]=0., Tayl = 0.893552 + 544.51 k_y^2

(kernel 4) Δ_{nem} = 2.25. Binary search converged after 8 iterations.

(kernel 4) θ_{crit}=9.03906, det[Hes]=0., Tayl = 16.6685 + 451.938 k_y^2

(kernel 8) Δ_{nem} = 0.25. Binary search converged after 10 iterations.

(kernel 8) θ_{crit}=8.6582, det[Hes]=0., Tayl = -2.52023 + 534.12 k_y^2

(kernel 5) Δ_{nem} = 1.75. Binary search converged after 10 iterations.

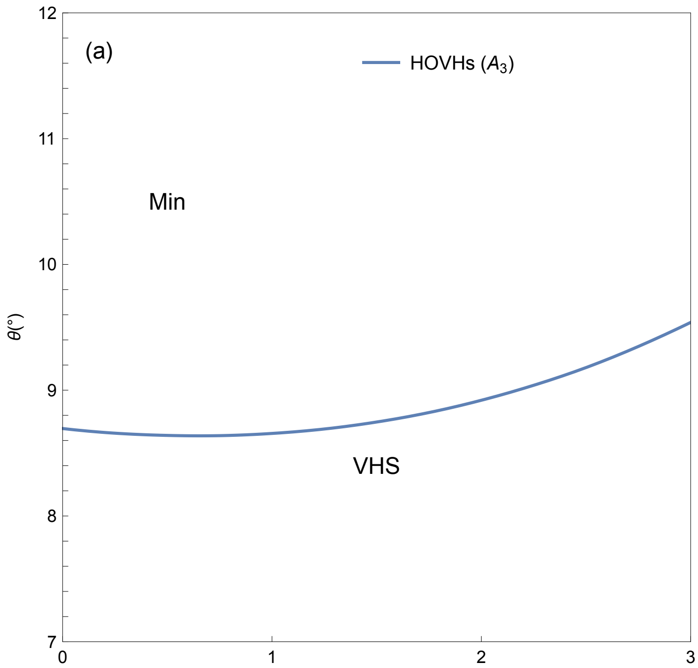
(kernel 5) θ_{crit}=8.82227, det[Hes]=0., Tayl = 10.0679 + 473.456 k_y^2

In[224]:=
```
HosListBand9p2 = SortBy[HosListBand9p2, First]
```

Out[224]=
```
{{0., 8.69531}, {0.25, 8.6582}, {0.5, 8.64063}, {0.75, 8.63867}, {1., 8.65625},
 {1.25, 8.69141}, {1.5, 8.74707}, {1.75, 8.82227}, {2., 8.91992},
 {2.25, 9.03906}, {2.5, 9.17969}, {2.75, 9.34766}, {3., 9.53906}}
```

In[643]:=
```
FitFunc3 = Interpolation[HosListBand9p2];
PlotBand9p2 = ListPlot[HosListBand9p2];
PanelA = Show[(*PlotBand9,*)Plot[FitFunc3[x], {x, 0, 3},
    FrameLabel → {(*"Δnem(%)"*)None, "θ(°)"}, PlotLegends → Placed[
      {Style["HOVHs (A3)", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
    PlotRange → {{0, 3}, {7, 12}}, Frame → True, AspectRatio → 1,
    FrameTicks → {{Automatic, None}, {{0, 1, 2, 3}, None}}],
  Graphics[Text[Style["VHS", FontFamily → "Arial", FontSize → 12], {1.5, 8.4}]],
  Graphics[Text[Style["Min", FontFamily → "Arial", FontSize → 12], {0.5, 10.5}]],
  Graphics[
   Text[Style["(a)", FontFamily → "Arial", FontSize → 12], {0.175, 11.7}]]]
```

Out[645]=



Band 8, part 2

In[243]:=
```
NoIterns = 5;
CurrResln = 10^-2;
```

```
kVHSTrialLow = {0, π - 0.9 × 3.869 × 0.35};
kVHSTrialUp = {0, π - 0.5 × 3.869 × 0.35};

HosListBand8p2 = {};
SetSharedVariable[HosListBand8p2];

ParallelDo[
 HamCurr[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], k[[3]], Delt];

 NoTry = 0;
 HOSFound = False;
 HOSPossible = True;
 θmax = 11;
 θmin = 8;

 (*Print["Binary search initiated for Δnem = ",Delt];*)

 While[NoTry ≤ 18 && HOSFound == False && HOSPossible == True,
  HamCurrUp[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmax, Delt];
  HamCurrDown[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmin, Delt];

  (*We compute the Hessian determinant for θmax*)
  (*Finding true kVHS:*)
  {kVHSmax, CritPtFound} = LocateCriticalPoint[
    HamCurrUp, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
    "SanityChecks" → True, "MaxIterations" → 28, "Resolution" → 10^-2];

  TaylorPolyMax = TaylorExpandBand[HamCurrUp, kVHSmax, 8, 2, "Messages" → False];
  TaylorPolyMax = Chop[TaylorPolyMax, CurrResln];

  (*Print["kcrit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

  If[CritPtFound == False,
   HOSPossible = False;
   (*Print["Critical point not found for θmax at Δnem = ",Delt,"."];*)
  ];


  (*We now compute the Hessian determinant for θmin*)
  (*Finding true kVHS:*)
  {kVHSmin, CritPtFound} = LocateCriticalPoint[
    HamCurrDown, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
    "SanityChecks" → True, "MaxIterations" → 28, "Resolution" → 10^-2];
```

```
TaylorPolyMin =
 TaylorExpandBand[HamCurrDown, kVHSmin, 8, 2, "Messages" → False];
TaylorPolyMin = Chop[TaylorPolyMin, CurrResln];

(*Print["kcrit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

If[CritPtFound == False,
 HOSPossible = False;
 (*Print["Critical point not found for θmin at Δnem = ",Delt,"."];*)
];

(*Now we begin the binary search if the
 Hessian determinants computed above are opposite in sign*)
If[Sign[HesDetMax] == -Sign[HesDetMin] && HOSFound == False && HOSPossible == True,

 θmid = 0.5 (θmax + θmin);
 HamCurrMid[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], θmid, Delt];

 (*Finding true kVHS1:*)
 {kVHSmid, CritPtFound} = LocateCriticalPoint[
   HamCurrMid, kVHSTrialLow, kVHSTrialUp, 8, "Messages" → False,
   "SanityChecks" → True, "MaxIterations" → 28, "Resolution" → 10^-2];

 TaylorPolyMid =
  TaylorExpandBand[HamCurrMid, kVHSmid, 8, 2, "Messages" → False];
 TaylorPolyMid = Chop[TaylorPolyMid, CurrResln];

 (*Print["kcrit,max = ",kVHSmax,TaylorPolyMax[[1]]];*)

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

 If[CritPtFound == False,
  HOSPossible = False;
  (*Print["Critical point not found for θmid at Δnem = ",Delt,"."];*)
 ];


 If[Chop[HesDetMid, 1.] == 0,
  HOSFound = True;
  ,
  If[Sign[HesDetMid] == Sign[HesDetMax],
```

```
        θmax = θmid;
        ,
        If[Sign[HesDetMid] == Sign[HesDetMin],
         θmin = θmid;
        ]
       ]
      ];

      NoTry++;
      ,
      If[HOSFound == False,
       Print[Style["No HOS in the range!", Red]];
       HOSPossible = False;
      ]
     ];
    ];

    If[HOSFound == True,
     Print["Δnem = ", Delt,
      ". Binary search converged after ", NoTry, " iterations."];
     Print["θcrit=", θmid, ", det[Hes]=", HesDetMid,
      ", Tayl = ", Chop[Total[TaylorPolyMid[[1]]] /. {p1 → kx, p2 → ky}]];
     AppendTo[HosListBand8p2, {Delt, θmid}];
     ,
     Print[Style["No HOS in the range!", Red]];
    ];
    , {Delt, 0, 3, 0.25}]
```

(kernel 8) Δ_{nem} = 0.. Binary search converged after 7 iterations.

(kernel 8) θ_{crit}=8.91406, det[Hes]=0., Tayl = $-11.6625 - 401.535\, k_y^2$

(kernel 6) Δ_{nem} = 1.. Binary search converged after 9 iterations.

(kernel 6) θ_{crit}=8.87305, det[Hes]=0., Tayl = $-4.07612 - 421.808\, k_y^2$

(kernel 1) Δ_{nem} = 3.. Binary search converged after 9 iterations.

(kernel 1) θ_{crit}=10.3965, det[Hes]=0., Tayl = $19.9354 - 377.913\, k_y^2$

(kernel 2) Δ_{nem} = 2.75. Binary search converged after 10 iterations.

(kernel 2) θ_{crit}=9.90723, det[Hes]=0., Tayl = $14.731 - 363.249\, k_y^2$

(kernel 3) Δ_{nem} = 2.5. Binary search converged after 10 iterations.

(kernel 3) θ_{crit}=9.61426, det[Hes]=0., Tayl = $10.644 - 356.736\, k_y^2$

(kernel 7) Δ_{nem} = 0.5. Binary search converged after 11 iterations.

(kernel 7) θ_{crit}=8.84229, det[Hes]=0., Tayl = $-7.58052 - 435.597\, k_y^2$

(kernel 4) Δ_{nem} = 2.. Binary search converged after 11 iterations.

(kernel 5) Δ_{nem} = 1.5. Binary search converged after 11 iterations.

(kernel 4) θ_{crit}=9.23779, det[Hes]=0., Tayl = $4.16252 - 360.735\, k_y^2$

(kernel 5) θ_{crit}=9.00342, det[Hes]=0., Tayl = -0.4611 - 385.693 k_y^2

(kernel 6) $\triangle_{nem}$ = 1.25. Binary search converged after 8 iterations.

(kernel 6) θ_{crit}=8.92578, det[Hes]=0., Tayl = -2.33688 - 403.661 k_y^2

(kernel 8) $\triangle_{nem}$ = 0.25. Binary search converged after 11 iterations.

(kernel 8) θ_{crit}=8.86572, det[Hes]=0., Tayl = -9.5228 - 423.674 k_y^2

(kernel 5) $\triangle_{nem}$ = 1.75. Binary search converged after 9 iterations.

(kernel 5) θ_{crit}=9.10742, det[Hes]=0., Tayl = 1.66954 - 370.75 k_y^2

(kernel 4) $\triangle_{nem}$ = 2.25. Binary search converged after 10 iterations.

(kernel 4) θ_{crit}=9.40332, det[Hes]=0., Tayl = 7.13174 - 356.105 k_y^2

(kernel 7) $\triangle_{nem}$ = 0.75. Binary search converged after 11 iterations.

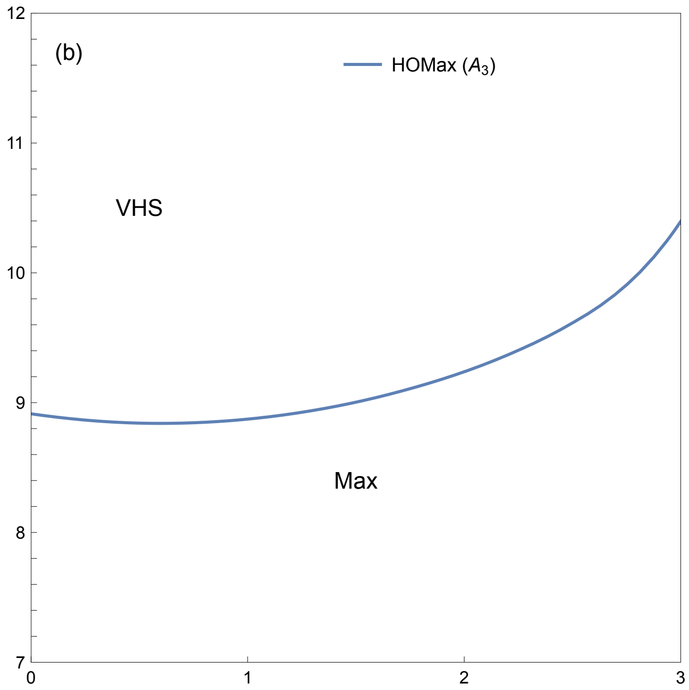
(kernel 7) θ_{crit}=8.84521, det[Hes]=0., Tayl = -5.79103 - 434.235 k_y^2

```
HosListBand8p2 = SortBy[HosListBand8p2, First]
```

Out[ ]= {{0., 8.91406}, {0.25, 8.88623}, {0.5, 8.88477}, {0.75, 8.90674}, {1., 8.95508}, {1.25, 9.02832}, {1.5, 9.12646}, {1.75, 9.24805}, {2., 9.39453}, {2.25, 9.57617}, {2.5, 9.80176}, {2.75, 10.1064}, {3., 10.5664}}

In[646]:=
```
FitFunc4 = Interpolation[HosListBand8p2];
PlotBand8p2 = ListPlot[HosListBand8p2];
PanelB = Show[(*PlotBand9,*)Plot[FitFunc4[x], {x, 0, 3},
   FrameLabel → {(*"Δnem(%)"*)None, (*"θ(°)"*)None}, PlotLegends → Placed[
     {Style["HOMax (A3)", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
   PlotRange → {{0, 3}, {7, 12}}, Frame → True, AspectRatio → 1,
   FrameTicks → {{Automatic, None}, {{0, 1, 2, 3}, None}}],
  Graphics[Text[Style["Max", FontFamily → "Arial", FontSize → 12], {1.5, 8.4}]],
  Graphics[Text[Style["VHS", FontFamily → "Arial", FontSize → 12], {0.5, 10.5}]],
  Graphics[
   Text[Style["(b)", FontFamily → "Arial", FontSize → 12], {0.175, 11.7}]]]
```

Out[648]=



Finding HOVHs at the M point

Bands 7 & 8

In[372]:=
```
HosListBand8M = {};
SetSharedVariable[HosListBand8M];

ParallelDo[
 HamCurr[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], k[[3]], Delt];

 θCurr = 9.5;
 CurrResln = 10^-2;
 HOSFound = False;
 NoTry = 1;
```

```
While[NoTry ≤ 4 && HOSFound == False,
 TaylorPoly =
  Chop[TaylorExpandBand[HamCurr(*The Hamiltonian*), {0, π // N, θCurr}
    (*the (k,t) point at which we are going to series expand.*), 8
    (*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}], CurrResln] == 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.*), 8
    (*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];

  Print["Δnem = ", Delt, "%. HOS found after ",
   NoTry, " iterations. θcrit = ", θCurr, ".\n\t Tayl = ",
   Total[Chop[ReplaceAll[TaylorPoly[[1]], {p1 → kx, p2 → ky, δθ → 0}], CurrResln]]];
  AppendTo[HosListBand8M, {Delt, θCurr}];
  ,
  Print[Style["No HOS found in the range!", Red]];
 ];

 , {Delt, 0, 3, 0.25}]
```

(kernel 6) Δ_{nem} = 1.%. HOS found after 1 iterations. θ_{crit} = 9.85442.
Tayl = $-16.0515 + 14.7302\,k_x^2 - 6.16167\,k_x^4 + 2.64509\,k_x^2\,k_y^2 - 98.8283\,k_y^4$

(kernel 3) Δ_{nem} = 2.5%. HOS found after 1 iterations. θ_{crit} = 10.676.
Tayl = $-1.1203 + 14.7639\,k_x^2 - 0.225672\,k_x^4 - 0.0179831\,k_x^3\,k_y - 5.33457\,k_x^2\,k_y^2 - 91.083\,k_y^4$

(kernel 4) Δ_{nem} = 2.%. HOS found after 1 iterations. θ_{crit} = 10.3027.
Tayl = $-6.92537 + 14.5612\,k_x^2 - 2.98365\,k_x^4 - 0.010227\,k_x^3\,k_y - 1.36728\,k_x^2\,k_y^2 - 95.0764\,k_y^4$

(kernel 7) Δ_{nem} = 0.5%. HOS found after 1 iterations. θ_{crit} = 9.78813.
Tayl = $-21.4024 + 14.8884\,k_x^2 - 6.00748\,k_x^4 + 1.98426\,k_x^2\,k_y^2 - 98.6179\,k_y^4$

(kernel 2) Δ_{nem} = 2.75%. HOS found after 1 iterations. θ_{crit} = 10.8872.
Tayl = $4.11285 + 15.0951\,k_x^2 +$
$1.19856\,k_x^4 - 0.0104415\,k_x^3\,k_y - 7.71679\,k_x^2\,k_y^2 - 88.1494\,k_y^4$

(kernel 5) Δ_{nem} = 1.5%. HOS found after 1 iterations. θ_{crit} = 10.0271.
Tayl = $-11.3397 + 14.6045\,k_x^2 - 5.04298\,k_x^4 + 1.31691\,k_x^2\,k_y^2 - 97.5853\,k_y^4$

(kernel 1) Δ_{nem} = 3.%. HOS found after 1 iterations. θ_{crit} = 11.0942.
Tayl = $12.1443 + 15.6561\,k_x^2 +$
$2.53934\,k_x^4 + 0.0126962\,k_x^3\,k_y - 10.2735\,k_x^2\,k_y^2 - 84.2225\,k_y^4$

(kernel 6) Δ_{nem} = 1.25%. HOS found after 1 iterations. θ_{crit} = 9.92773.
Tayl = $-13.6311 + 14.6612\,k_x^2 - 5.7261\,k_x^4 + 2.1578\,k_x^2\,k_y^2 - 98.3617\,k_y^4$

(kernel 8) Δ_{nem} = 0.%. HOS found after 1 iterations. θ_{crit} = 9.84004.
Tayl = $-27.6633 - 98.7668\,k_x^4 + 15.2032\,k_y^2 + 4.52407\,k_x^2\,k_y^2 - 8.08155\,k_y^4$

(kernel 4) Δ_{nem} = 2.25%. HOS found after 1 iterations. θ_{crit} = 10.4782.
Tayl = $-4.45347 + 14.6106\,k_x^2 - 1.65792\,k_x^4 - 0.0156096\,k_x^3\,k_y - 3.2007\,k_x^2\,k_y^2 - 93.3075\,k_y^4$

(kernel 7) Δ_{nem} = 0.75%. HOS found after 1 iterations. θ_{crit} = 9.80776.
Tayl = $-18.6317 + 14.8069\,k_x^2 - 6.30955\,k_x^4 + 2.69655\,k_x^2\,k_y^2 - 98.9632\,k_y^4$

(kernel 5) Δ_{nem} = 1.75%. HOS found after 1 iterations. θ_{crit} = 10.1522.
Tayl = $-9.13606 + 14.5672\,k_x^2 - 4.12422\,k_x^4 + 0.140926\,k_x^2\,k_y^2 - 96.4934\,k_y^4$

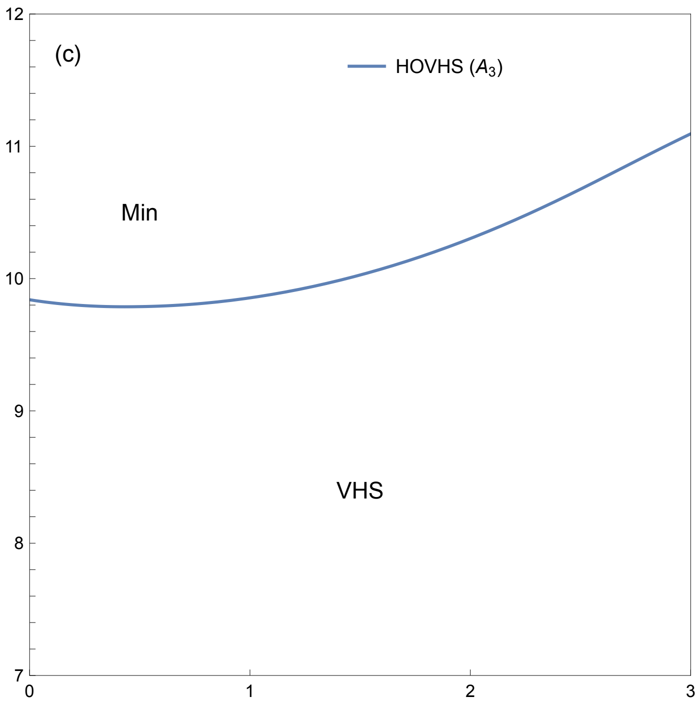
(kernel 8) Δ_{nem} = 0.25%. HOS found after 1 iterations. θ_{crit} = 9.79559.
Tayl = $-24.3922 + 14.9735\,k_x^2 - 4.34226\,k_x^4 - 1.32057\,k_x^2\,k_y^2 - 96.8826\,k_y^4$

In[379]:=
```
HosListBand8M = SortBy[HosListBand8M, First]
```

Out[379]=
```
{{0., 9.84004}, {0.25, 9.79559}, {0.5, 9.78813}, {0.75, 9.80776},
 {1., 9.85442}, {1.25, 9.92773}, {1.5, 10.0271}, {1.75, 10.1522},
 {2., 10.3027}, {2.25, 10.4782}, {2.5, 10.676}, {2.75, 10.8872}, {3., 11.0942}}
```

In[649]:=
```
FitFunc5 = Interpolation[HosListBand8M];
PlotBand8p3 = ListPlot[HosListBand8M, AxesLabel → {"Δnem (%)", "θ(°)"},
   PlotLegends → Placed[{"HOVHs (A3)"}, {0.5, 0.965}]];
PanelC = Show[(*PlotBand9,*)Plot[FitFunc5[x], {x, 0, 3},
   FrameLabel → {(*"Δnem (%)","θ(°)"*)None, None}, PlotLegends → Placed[
     {Style["HOVHS (A3)", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
   PlotRange → {{0, 3}, {7, 12}}, Frame → True, AspectRatio → 1,
   FrameTicks → {{Automatic, None}, {{0, 1, 2, 3}, None}}],
  Graphics[Text[Style["VHS", FontFamily → "Arial", FontSize → 12], {1.5, 8.4}]],
  Graphics[Text[Style["Min", FontFamily → "Arial", FontSize → 12], {0.5, 10.5}]],
  Graphics[
   Text[Style["(c)", FontFamily → "Arial", FontSize → 12], {0.175, 11.7}]]]
```

Out[651]=



Bands 9 & 10

In[361]:=
```
HosListBand6M = {};
SetSharedVariable[HosListBand6M];

ParallelDo[
 HamCurr[k_] := HamiltonianNemTunedmeV[k[[1]], k[[2]], k[[3]], Delt];

 θCurr = 9.5;
 CurrResln = 10^-2;
```

```
HOSFound = False;
NoTry = 1;

While[NoTry ≤ 4 && HOSFound == False,
 TaylorPoly =
  Chop[TaylorExpandBand[HamCurr(*The Hamiltonian*), {0, π // N, θCurr}
    (*the (k,t) point at which we are going to series expand.*), 6
    (*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}], CurrResln] == 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.*), 6
    (*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];

  Print["Δnem = ", Delt, "%. HOS found after ",
   NoTry, " iterations. θcrit = ", θCurr, ".\n\t Tayl = ",
   Total[Chop[ReplaceAll[TaylorPoly[[1]], {p1 → kx, p2 → ky, δθ → 0}], CurrResln]]];
  AppendTo[HosListBand6M, {Delt, θCurr}];
  ,
  Print[Style["No HOS found in the range!", Red]];
 ];

, {Delt, 0, 3, 0.25}]
```

(kernel 6) Δ_{nem} = 1.%. HOS found after 1 iterations. θ_{crit} = 9.80565.
Tayl = $-18.3115 - 100.389\, k_x^4 + 15.3957\, k_y^2 + 6.3958\, k_x^2 k_y^2 - 8.19816\, k_y^4$

(kernel 3) Δ_{nem} = 2.5%. HOS found after 1 iterations. θ_{crit} = 10.5276.
Tayl =
$-7.08976 - 96.3126\, k_x^4 + 0.0304409\, k_x^3 k_y + 16.292\, k_y^2 + 7.01689\, k_x^2 k_y^2 - 0.015326\, k_x k_y^3 - 6.81202\, k_y^4$

(kernel 4) Δ_{nem} = 2.%. HOS found after 1 iterations. θ_{crit} = 10.1907.
Tayl =
$-11.2329 - 98.1961\, k_x^4 + 0.0167324\, k_x^3 k_y + 15.8689\, k_y^2 + 6.43314\, k_x^2 k_y^2 - 0.0122696\, k_x k_y^3 - 7.26008\, k_y^4$

(kernel 2) Δ_{nem} = 2.75%. HOS found after 1 iterations. θ_{crit} = 10.7272.
Tayl =
$-3.57871 - 95.0433\, k_x^4 + 0.0288984\, k_x^3 k_y + 16.6474\, k_y^2 + 7.59568\, k_x^2 k_y^2 - 0.0122503\, k_x k_y^3 - 6.80334\, k_y^4$

(kernel 7) Δ_{nem} = 0.5%. HOS found after 1 iterations. θ_{crit} = 9.76426.
Tayl = $-22.5278 - 101.247\, k_x^4 + 15.2214\, k_y^2 + 7.54739\, k_x^2 k_y^2 - 8.86719\, k_y^4$

(kernel 5) Δ_{nem} = 1.5%. HOS found after 1 iterations. θ_{crit} = 9.94961.
Tayl = $-14.6564 - 99.5305\, k_x^4 + 15.5997\, k_y^2 + 6.24236\, k_x^2 k_y^2 - 7.76804\, k_y^4$

(kernel 1) Δ_{nem} = 3.%. HOS found after 1 iterations. θ_{crit} = 10.9341.
Tayl = $2.19695 - 93.3049\, k_x^4 +$
$0.0105083\, k_x^3 k_y + 17.1833\, k_y^2 + 8.54108\, k_x^2 k_y^2 - 7.12536\, k_y^4$

(kernel 6) Δ_{nem} = 1.25%. HOS found after 1 iterations. θ_{crit} = 9.86521.
Tayl = $-16.4337 - 100.007\, k_x^4 + 15.4922\, k_y^2 + 6.26773\, k_x^2 k_y^2 - 7.98998\, k_y^4$

(kernel 8) Δ_{nem} = 0.%. HOS found after 1 iterations. θ_{crit} = 9.84004.
Tayl = $-27.6633 - 98.7668\, k_x^4 + 15.2032\, k_y^2 + 4.52407\, k_x^2 k_y^2 - 8.08155\, k_y^4$

(kernel 4) Δ_{nem} = 2.25%. HOS found after 1 iterations. θ_{crit} = 10.3474.
Tayl =
$-9.39628 - 97.3302\, k_x^4 + 0.0242414\, k_x^3 k_y + 16.0497\, k_y^2 + 6.66007\, k_x^2 k_y^2 - 0.0146498\, k_x k_y^3 - 7.00332\, k_y^4$

(kernel 7) Δ_{nem} = 0.75%. HOS found after 1 iterations. θ_{crit} = 9.77175.
Tayl = $-20.3288 - 100.741\, k_x^4 + 15.3063\, k_y^2 + 6.71231\, k_x^2 k_y^2 - 8.43553\, k_y^4$

(kernel 5) Δ_{nem} = 1.75%. HOS found after 1 iterations. θ_{crit} = 10.0582.
Tayl = $-12.9416 - 98.9297\, k_x^4 + 0.0105295\, k_x^3 k_y + 15.723\, k_y^2 + 6.29789\, k_x^2 k_y^2 - 7.52287\, k_y^4$

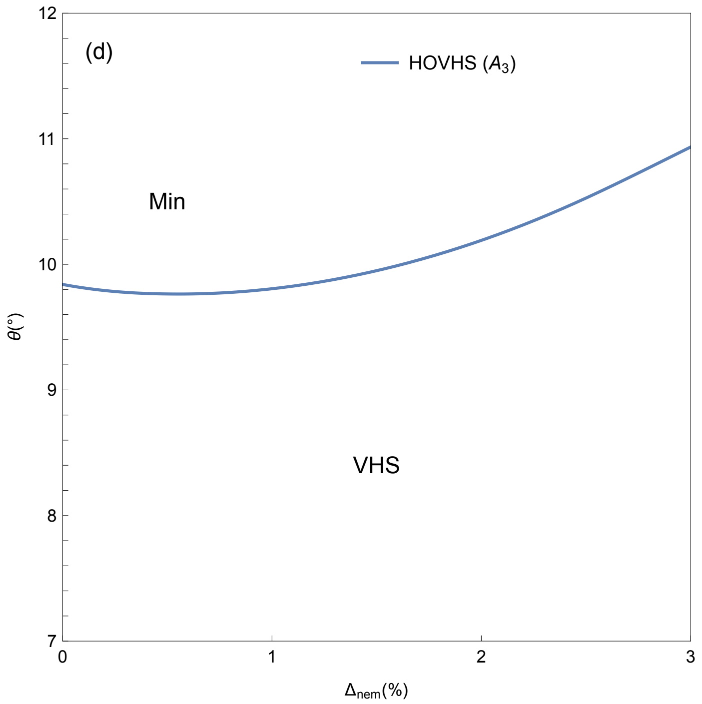
(kernel 8) Δ_{nem} = 0.25%. HOS found after 1 iterations. θ_{crit} = 9.78358.
Tayl = $-24.9486 - 102.832\, k_x^4 + 15.14\, k_y^2 + 10.7305\, k_x^2 k_y^2 - 10.4072\, k_y^4$

In[375]:=
```
HosListBand6M = SortBy[HosListBand6M, First]
```

Out[375]=
```
{{0., 9.84004}, {0.25, 9.78358}, {0.5, 9.76426}, {0.75, 9.77175}, {1., 9.80565},
 {1.25, 9.86521}, {1.5, 9.94961}, {1.75, 10.0582}, {2., 10.1907},
 {2.25, 10.3474}, {2.5, 10.5276}, {2.75, 10.7272}, {3., 10.9341}}
```

In[652]:=
```
FitFunc6 = Interpolation[HosListBand6M];
PlotBand6 = ListPlot[HosListBand6M, AxesLabel → {"Δnem (%)", "θ(°)"},
   PlotLegends → Placed[{"HOVHs (A3)"}, {0.5, 0.965}]];
PanelD = Show[(*PlotBand9,*)Plot[FitFunc6[x],
   {x, 0, 3}, FrameLabel → {"Δnem (%)", "θ(°)"}, PlotLegends → Placed[
     {Style["HOVHS (A3)", FontFamily → "Arial", FontSize → 10]}, {0.6, 0.92}],
   PlotRange → {{0, 3}, {7, 12}}, Frame → True, AspectRatio → 1,
   FrameTicks → {{Automatic, None}, {{0, 1, 2, 3}, None}}],
  Graphics[Text[Style["VHS", FontFamily → "Arial", FontSize → 12], {1.5, 8.4}]],
  Graphics[Text[Style["Min", FontFamily → "Arial", FontSize → 12], {0.5, 10.5}]],
  Graphics[
   Text[Style["(d)", FontFamily → "Arial", FontSize → 12], {0.175, 11.7}]]]
```

Out[654]=



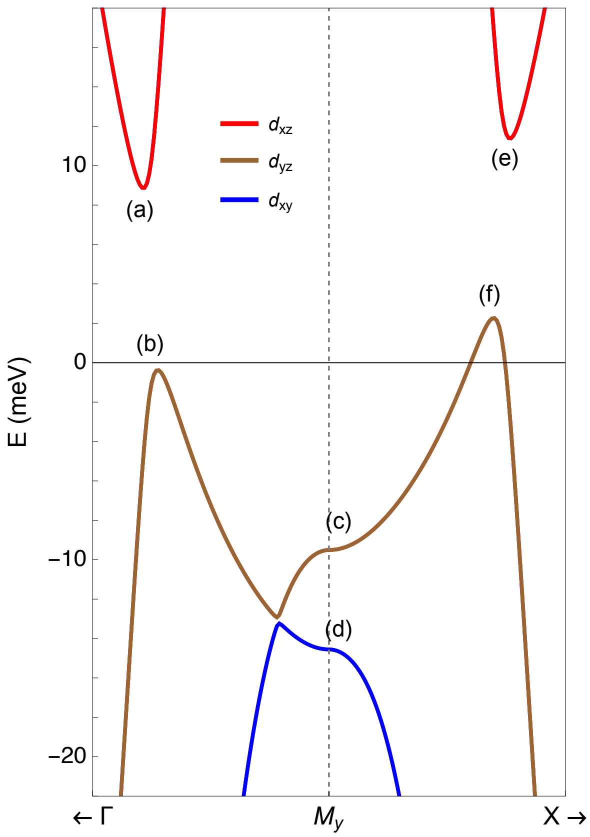
Assembling the results

Labeling the critical points of interest

```
Bnd4 = GenerateBandStructure[HamTempNem2, HSymmPts, "OrbitalProjection" → True,
   "OrbitalGrouping" → {{1, 4, 7, 10}, {2, 5, 8, 11}, {3, 6, 9, 12}}];
```

```
In[656]:= PltCritPts =
  PlotBandStructure[Bnd3, (*{-0.042,0.012}*){-22, 18}, AspectRatio → 5/3,
   "yLabel" → {(*Label*)"E (meV)", (*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, 0.8}}];
PanelCritPts = Show[PltCritPts,
  Graphics[Text[Style["(a)", FontFamily → "Arial", FontSize → 12], {0.28, 7.8}]],
  Graphics[Text[Style["(b)", FontFamily → "Arial", FontSize → 12], {0.34, 1}]],
  Graphics[Text[Style["(c)", FontFamily → "Arial", FontSize → 12], {1.45, -8}]],
  Graphics[Text[Style["(d)", FontFamily → "Arial", FontSize → 12],
    {1.45, -13.5}]], Graphics[
   Text[Style["(e)", FontFamily → "Arial", FontSize → 12], {2.43, 10.42}]],
  Graphics[Text[Style["(f)", FontFamily → "Arial", FontSize → 12], {2.34, 3.5}]]]
```

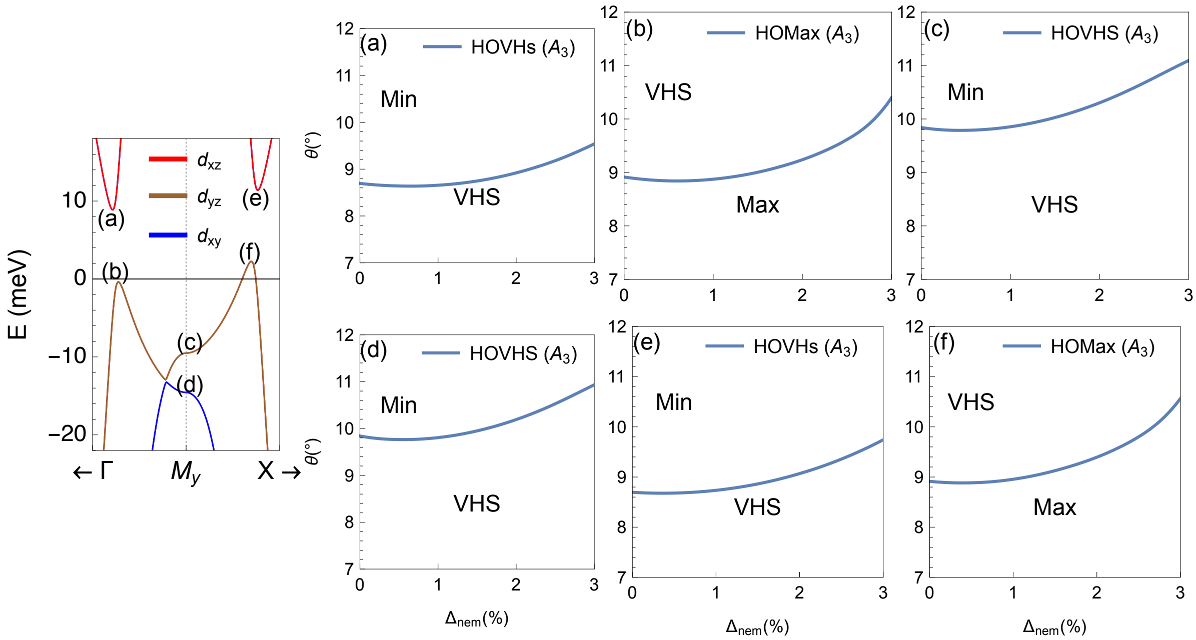
Out[657]=



Phase diagrams for the critical points

In[658]:=
```
Show[GraphicsGrid[{{PanelCritPts, PanelA, PanelB, PanelC},
   {SpanFromAbove, PanelD, PanelE, PanelF}},
  Spacings → {Scaled[0.], Scaled[0.02]}, ImageSize → Full]
```

Out[658]=



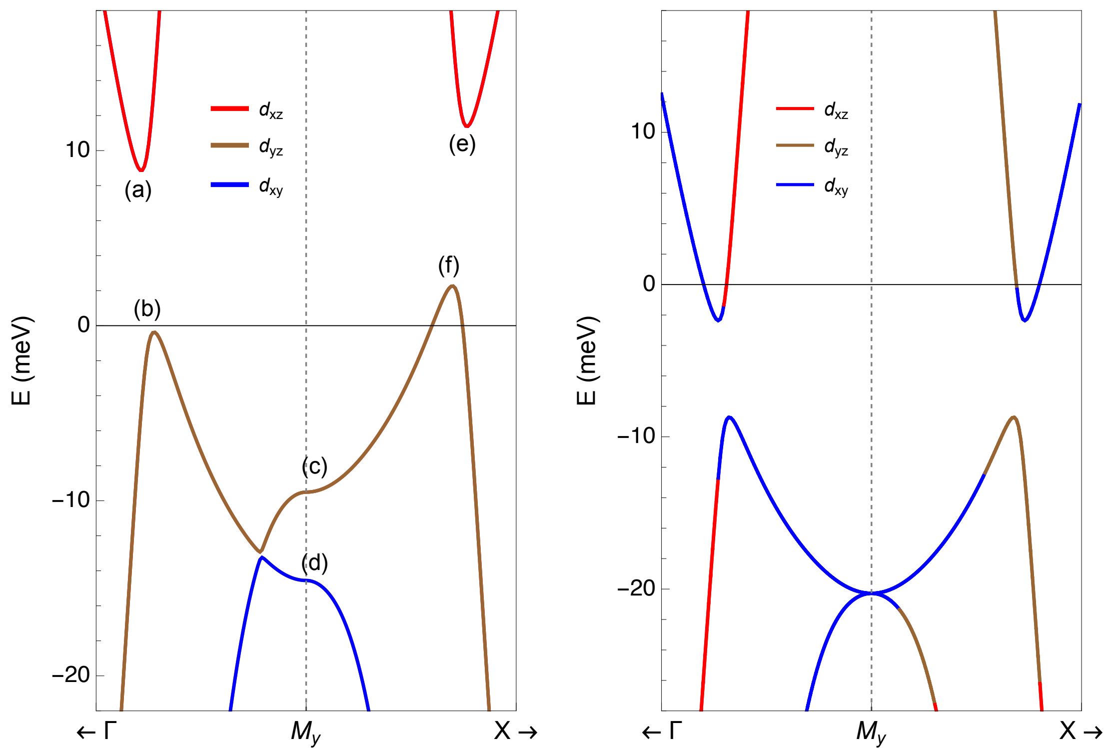
We can also examine the orbital-projected band structure in the absence of nematicity and compare with the nematic model

In[419]:=
```
BndTemp = GenerateBandStructure[HamTemp, HSymmPts, "OrbitalProjection" → True,
   "OrbitalGrouping" → {{1, 4, 7, 10}, {2, 5, 8, 11}, {3, 6, 9, 12}}];
```

In[659]:=
```
PltTemp =
  PlotBandStructure[BndTemp, (*{-0.042,0.012}*){-28, 18}, AspectRatio → 5/3,
   "yLabel" → {(*Label*)"E  (meV)", (*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, 0.8}}];
```

In[660]:=
```
GraphicsRow[{PanelCritPts, PltTemp}]
```

Out[660]=



The dominant orbitals seem to have changed. (Note that we have computed the total contribution of each type of orbital across both the Ru atoms and both spin species).

Phase diagrams

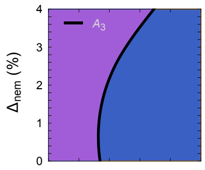
We will now generate the phase diagram for the SOC gap singularities that is included in the manuscript

In[421]:=
```
θmin = 7;
θmax = 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};
```

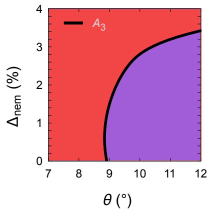
```
VHsColour = {(*125*)161/255, (*9*)93/255, (*184*)216/255, 1(*0.65*)};
MinColour = {(*9*)59/255, (*73*)96/255, (*184*)196/255, 1(*0.65*)};
MaxColour = {(*207*)242/255, (*17*)70/255, (*51*)70/255, 1(*0.65*)};

PanA = ParametricPlot[
   {{v FitFunc3[u] + θmin (1 - v), u}, {(1 - v) FitFunc3[u] + θmax v, u}},
   {u, 0, 4}, {v, 0, 1}, PlotRange → {{θmin, θmax}, {0, 4}}, Frame → True,
   PlotStyle → {RGBColor[VHsColour], RGBColor[MinColour]}, AspectRatio → 1,
   (*FrameTicks→{True,True},*)(*FrameLabel→{None,Style["Δnem (%)",
      FontFamily→"Arial",FontSize→AxesFontSize,FontColor→Black]},*)
   FrameTicksStyle → {Directive[Black, FontFamily → "Arial", TicsFontSize],
     {Directive[FontOpacity → 0, FontSize → 0], Directive[FontOpacity → 0,
       FontSize → 0]}}, FrameTicks → {True, {xTics, xTics}},
   ImagePadding → {{LeftPadding, RightPadding}, {0.6 TopPadding, TopPadding}},
   ImageSize → FigLength];

PanAp2 = ParametricPlot[{FitFunc3[u], u}, {u, 0, 4}, Axes → False, Frame → False,
   PlotStyle → {Black, Thickness[0.018]}, PlotRange → {{θmin, θmax}, {0, 4}},
   PlotLegends → Placed[LineLegend[{Style["A3", FontFamily → "Arial",
         FontSize → TicsFontSize, FontColor → RegionFontColour]},
      LegendMarkerSize → {10, 1.3}], {{0.25, 0.92}, {0.5, 0.5}}]];

Labeled[Show[PanA, PanAp2], {Style["Δnem (%)",
   FontFamily → "Arial", FontSize → AxesFontSize, FontColor → Black], ""},
 {Left, Bottom}, Spacings → {0, 0}, RotateLabel → True]


PanB = ParametricPlot[
   {{v FitFunc4[u] + θmin (1 - v), u}, {(1 - v) FitFunc4[u] + θmax v, u}},
   {u, 0, 4}, {v, 0, 1}, PlotRange → {{θmin, θmax}, {0, 4}}, Frame → True,
   PlotStyle → {RGBColor[MaxColour], RGBColor[VHsColour]}, AspectRatio → 1,
   FrameTicksStyle → {Directive[Black, FontFamily → "Arial", TicsFontSize],
     {Directive[Black, FontFamily → "Arial", TicsFontSize],
      Directive[FontOpacity → 0, FontSize → 0]}},
   FrameTicks → {True, {xTicsLabeled, xTics}}, ImagePadding →
    {{LeftPadding, RightPadding}, {BottomPadding, 0.5 TopPadding}},
   ImageSize → FigLength];

PanBp2 = ParametricPlot[{FitFunc4[u], u}, {u, 0, 4},
   Axes → False, Frame → False, PlotStyle → {Black, Thickness[0.018]},
   PlotLegends → Placed[LineLegend[{Style["A3", FontFamily → "Arial",
         FontSize → TicsFontSize, FontColor → RegionFontColour]},
      LegendMarkerSize → {10, 1.3}], {{0.25, 0.92}, {0.5, 0.5}}]];
```

```
Labeled[Show[PanB, PanBp2],
 {Style["Δnem (%)", FontFamily → "Arial", FontSize → AxesFontSize,
   FontColor → Black], Style["θ (°)", FontFamily → "Arial",
   FontSize → AxesFontSize, FontColor → Black]},
 {Left, Bottom}, Spacings → {0, 0}, RotateLabel → True]
```

Out[439]=

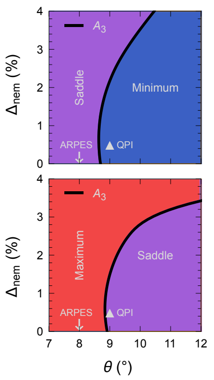


Out[442]=



In[443]:=
```
PhaseDiagramFinal =
 GraphicsGrid[{{Labeled[Show[PanA, PanAp2, Graphics[Rotate[Text[
         Style["Saddle", FontFamily → "Arial", FontColor → RegionFontColour,
          FontSize → TicsFontSize], {8, 2}], 90 Degree]], Graphics[
      Text[Style["Minimum", FontFamily → "Arial", FontColor → RegionFontColour,
         FontSize → TicsFontSize], {10.5, 2.0}]], ListPlot[{{9, 0.5}},
      PlotMarkers → {▲, 2.5}, PlotStyle → {LightGray, Thickness[0.02]}],
     Graphics[Text[Style["QPI", FontFamily → "Arial", FontColor →
          RegionFontColour, FontSize → (TicsFontSize - 1)], {9.5, 0.45}]],
     ListPlot[{{8, 0.16}}, PlotMarkers → {"↓", 8}, PlotStyle → {LightGray}],
     Graphics[Text[Style["ARPES", FontFamily → "Arial", FontColor →
          RegionFontColour, FontSize → (TicsFontSize - 1)], {7.9, 0.5}]]],
    {Style["Δnem (%)", FontFamily → "Arial", FontSize → AxesFontSize,
      FontColor → Black]}, {Left}, Spacings → {0.1, 0}, RotateLabel → True]
  }, {Labeled[Show[PanB, PanBp2,
     Graphics[Rotate[Text[Style["Maximum", FontFamily → "Arial", FontColor →
           RegionFontColour, FontSize → TicsFontSize], {8, 2}], 90 Degree]],
     Graphics[Text[Style["Saddle", FontFamily → "Arial",
        FontColor → RegionFontColour, FontSize → TicsFontSize], {10.5, 2.0}]],
     ListPlot[{{9, 0.5}}, PlotMarkers → {▲, 2.5},
      PlotStyle → {LightGray, Thickness[0.02]}],
     Graphics[Text[Style["QPI", FontFamily → "Arial", FontColor →
          RegionFontColour, FontSize → (TicsFontSize - 1)], {9.5, 0.45}]],
     ListPlot[{{8, 0.16}}, PlotMarkers → {"↓", 8}, PlotStyle → {LightGray}],
     Graphics[Text[Style["ARPES", FontFamily → "Arial", FontColor →
          RegionFontColour, FontSize → (TicsFontSize - 1)], {7.9, 0.5}]]],
    {Style["Δnem (%)", FontFamily → "Arial", FontSize → AxesFontSize,
      FontColor → Black], Style["θ (°)", FontFamily → "Arial",
      FontSize → AxesFontSize, FontColor → Black]}, {Left, Bottom},
    Spacings → {0.1, 0}, RotateLabel → True]}}, Spacings → {0, -8}]

Export[NotebookDirectory[] <> "Phase_horiz.pdf",
 Show[PhaseDiagramFinal, ImageSize → 4.5 cm]]
```

Out[443]=



Out[444]= /Users/phac/Research/GitHub/BandUtilities/Sr2RuO4/Phase_horiz.pdf