

```
In[*]:= Charting`$InteractiveHighlighting = False
Out[*]:=
False
```

Coarse mesh with 14 samples

```
In[*]:= data =
  Dataset[Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
    Documents/com~apple~CloudDocs/LM
    MANO/Computational material physics /Cluster
    data/P2/output02/output``.csv", #], "Table",
    "HeaderLines" → 0, "FieldSeparators" → "\t", "NumberPoint" → ".",
    CharacterEncoding → "UTF8"]][All, Range[1, 11]][All,
  Rule@@@Transpose[{ToString@StringForm["Band ``", #] & /@ Range[1, 11] //
    Evaluate, Range[1, 11]}] // Association] & /@ {"Up", "Down"};

In[*]:= data2 = Table[Transpose[
  {Range[0.75, 4, 0.25], di[All, ToString@StringForm["Band ``", #]]} //
  Normal] & /@ Range[1, 11], {di, data}];

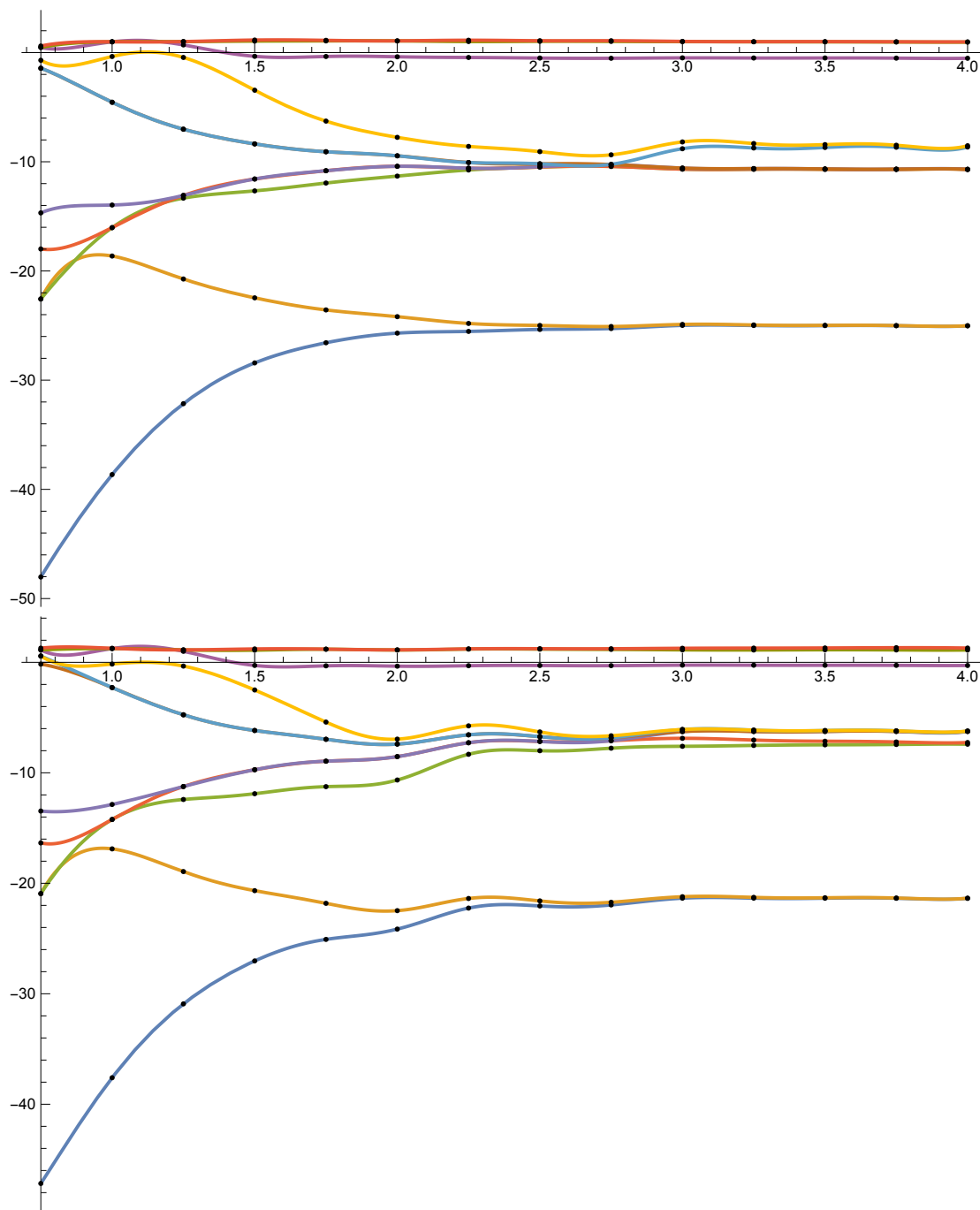
In[*]:= Range[0.75, 4, 0.25] // Length
Out[*]:=
14
```

```

In[*]:= Table[Interpolation[#, InterpolationOrder → 5, Method → "Spline"][d] & /@ di //
  Plot[#, {d, 0.75, 4}, ImageSize → Large, Epilog → {Point[#] & /@ di},
    PlotRange → All] &, {di, data2}] // TableForm

```

Out[*]//TableForm=



```

In[*]:= data =
  Dataset[Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
    Documents/com~apple~CloudDocs/LM MANO/Computational material
    physics /Cluster data/P2/output02/outputETOT.csv"], "Table",
    "HeaderLines" → 0, "FieldSeparators" → "\t", "NumberPoint" → ".",
    CharacterEncoding → "UTF8"]][All, Range[1, 1]][All,
    Rule@@@Transpose[{ToString@StringForm["Band ``", #] & /@Range[1, 1] //
      Evaluate, Range[1, 1]}] // Association]

```

Out[*]=

Band 1
24.4871
-6.15164
-9.83918
-8.4155
-6.39093
-4.68474
-4.23425
-3.94909
-3.70156
-3.72284
-3.75421
-3.76573
-3.76886
-3.77241

```

In[*]:= data2 = Transpose[
  {Range[0.75, 4, 0.25], data[All, ToString@StringForm["Band ``", #]]} //
  Normal] & /@Range[1, 1] // First

```

Out[*]=

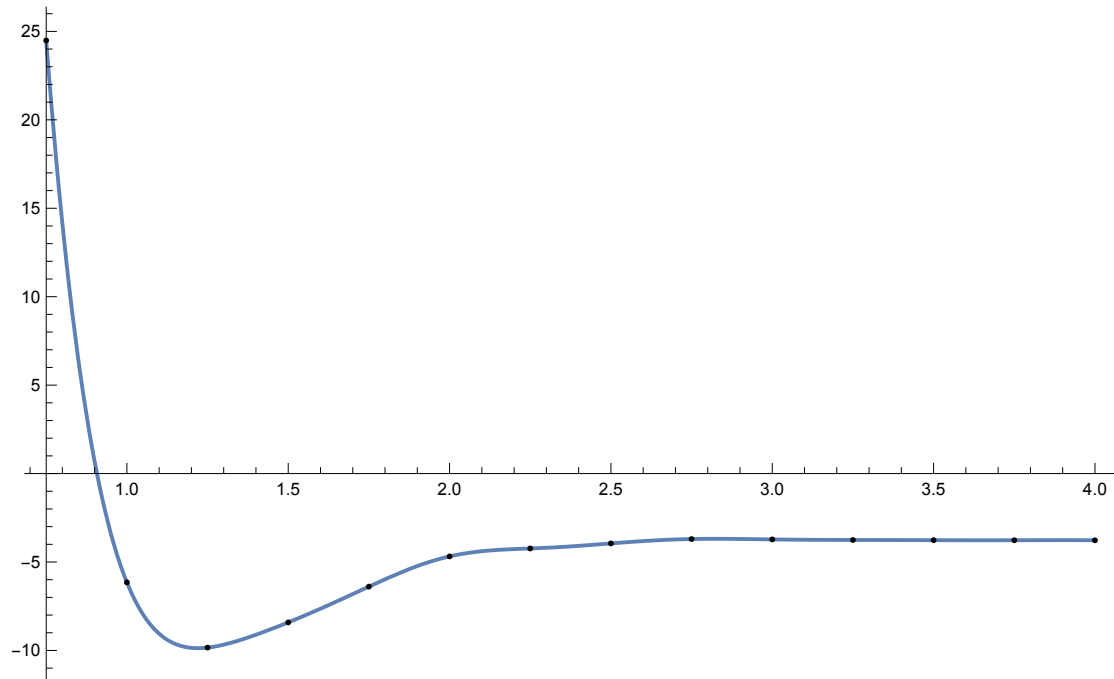
```

{{0.75, 24.4871}, {1., -6.15164}, {1.25, -9.83918},
 {1.5, -8.4155}, {1.75, -6.39093}, {2., -4.68474}, {2.25, -4.23425},
 {2.5, -3.94909}, {2.75, -3.70156}, {3., -3.72284},
 {3.25, -3.75421}, {3.5, -3.76573}, {3.75, -3.76886}, {4., -3.77241}}

```

```
In[*]:= Interpolation[data2, InterpolationOrder → 5, Method → "Spline"][d] //
Plot[#, {d, 0.75, 4}, ImageSize → Large,
Epilog → {Point[#] & /@ data2}, PlotRange → All] &
```

Out[*]=



```
In[*]:= ListLinePlot[data2, PlotRange → All, ImageSize → Large]
```

Finer mesh with 80 samples

```
In[*]:= data =
Dataset[Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
Documents/com~apple~CloudDocs/LM
MANO/Computational material physics /Cluster
data/P2/output02/output``.csv", #], "Table",
"HeaderLines" → 0, "FieldSeparators" → "\t", "NumberPoint" → ".",
CharacterEncoding → "UTF8"]][All, Range[1, 11]][All,
Rule@@@Transpose[{ToString@StringForm["Band ``", #] & /@ Range[1, 11] //
Evaluate, Range[1, 11]}] // Association] & /@ {"FineUp", "FineDown"};
```

```
In[*]:= data = Table[Transpose[
{Range[0.05, 4.0, 0.05], di[All, ToString@StringForm["Band ``", #]]} //
Normal] & /@ Range[1, 11], {di, data}];
```

```
In[*]:= Range[0.05, 4.0, 0.05] // Length
```

Out[*]=

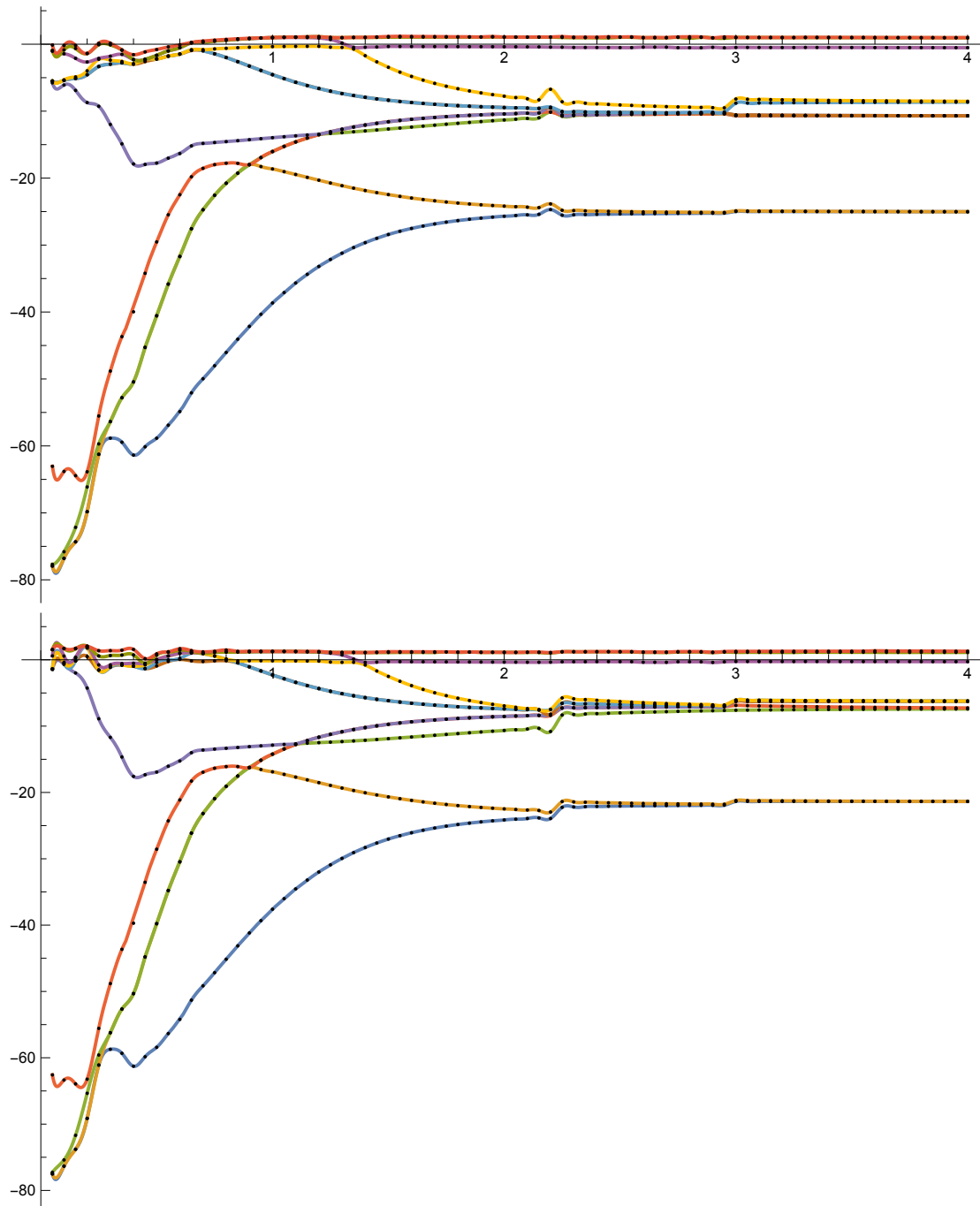
80

```

In[*]:= Table[Interpolation[#, InterpolationOrder → 5, Method → "Spline"][d] & /@ di //
  Plot[#, {d, 0.05, 4}, Epilog → {PointSize[Small], Point[#] & /@ di},
    ImageSize → Large, PlotRange → All] &, {di, data}] // TableForm

```

Out[*]//TableForm=



Ultra-fine mesh with 400 samples

```

In[*]:= data =
  Dataset[Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
    Documents/com~apple~CloudDocs/LM
    MANO/Computational material physics /Cluster
    data/P2/output02/output``.csv", #], "Table",
    "HeaderLines" → 0, "FieldSeparators" → "\t", "NumberPoint" → ".",
    CharacterEncoding → "UTF8"]][All, Range[1, 11]][
  All, Rule @@@ Transpose[{ToString@StringForm["Band ``", #] & /@
    Range[1, 11] // Evaluate, Range[1, 11]}] //
  Association] & /@ {"UltraFineUp", "UltraFineDown"};

In[*]:= data = Table[Transpose[
  {Range[0.01, 4.0, 0.01], di[All, ToString@StringForm["Band ``", #]]} //
  Normal] & /@ Range[1, 11], {di, data}];

In[*]:= Range[0.01, 4.0, 0.01] // Length
Out[*]=
  400

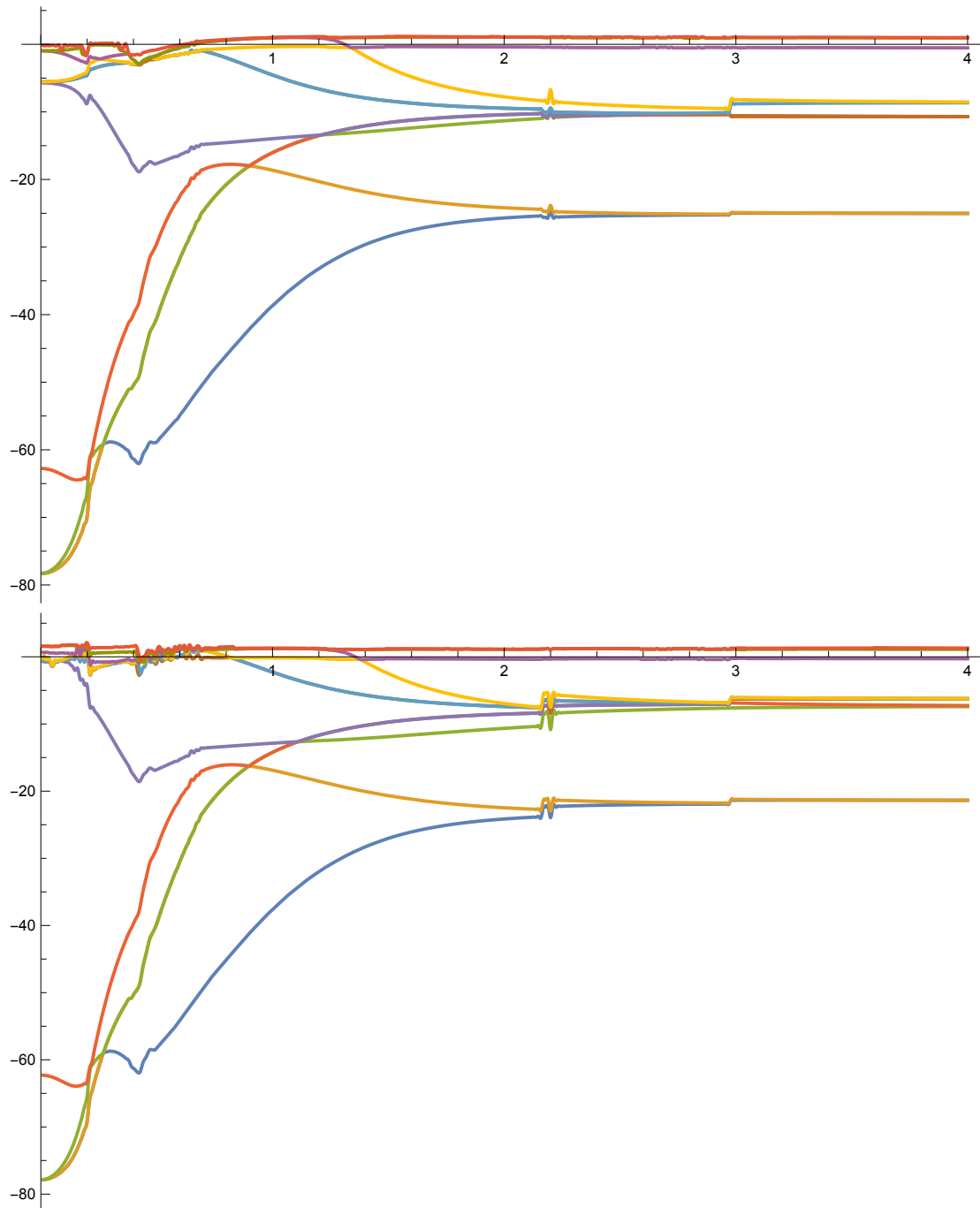
```

```

In[*]:= Table[Interpolation[#, InterpolationOrder → 5, Method → "Spline"] [d] & /@ di //
  Plot[#, {d, 0.01, 4}, ImageSize → Large, PlotRange → All] &,
  {di, data}] // TableForm

```

Out[*]//TableForm=

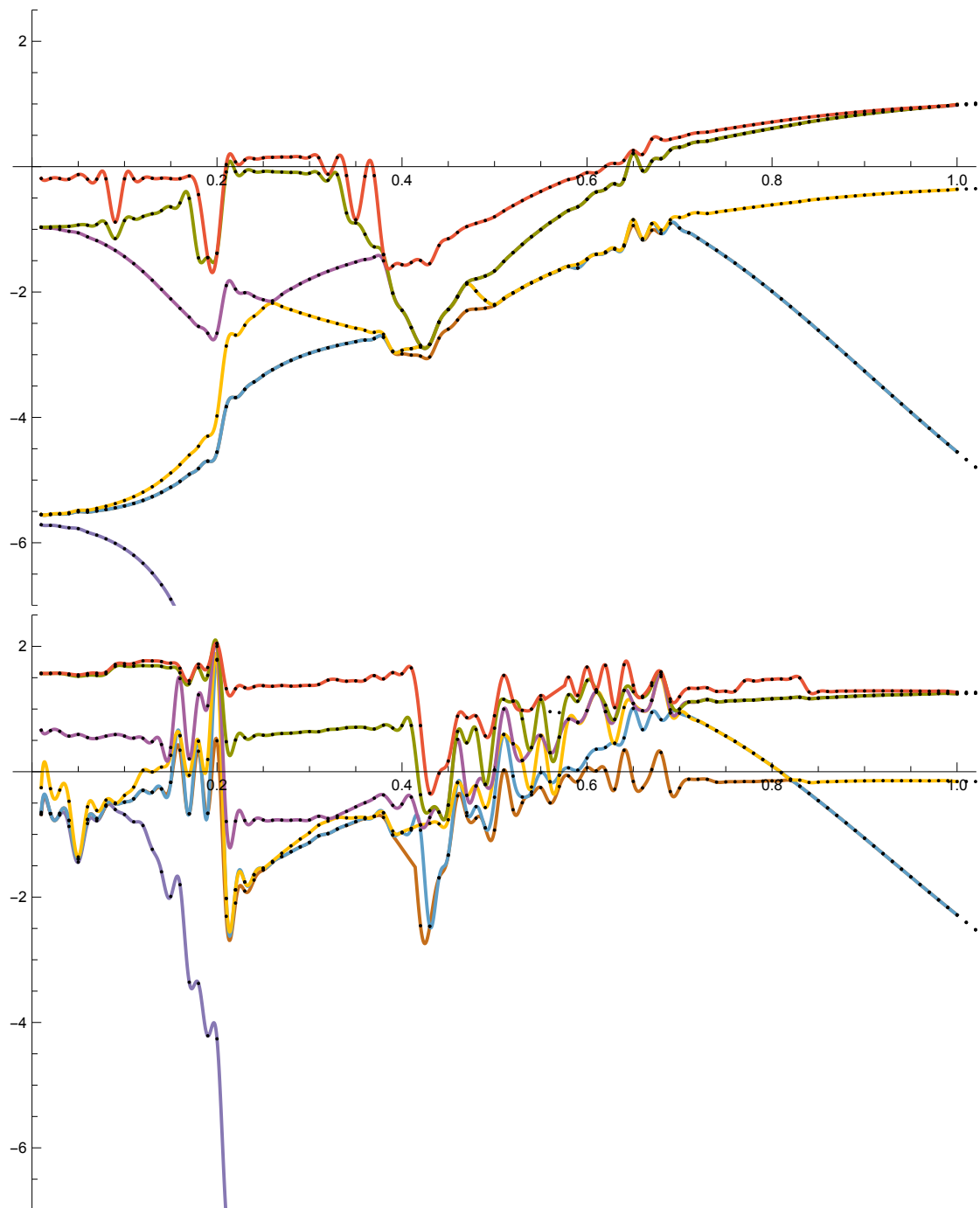


```

In[*]:= Table[Interpolation[#, InterpolationOrder → 5, Method → "Spline"][d] & /@ di //
  Plot[#, {d, 0.01, 1}, Epilog → {PointSize[Small], Point[#] & /@ di},
    ImageSize → Large, PlotRange → {-7, 2.5}] &, {di, data}] // TableForm

```

Out[*] // TableForm =



Mega-zoom into the interval $[0, 1]$ with 1000 samples

```

In[*]:= Range[0.001, 1.0, 0.001] // Length

```

Out[*] =

1000


```

In[*]:= data =
  Dataset[Import[ToString@StringForm["/Users/giovannigravili/Library/Mobile
    Documents/com~apple~CloudDocs/LM
    MAN0/Computational material physics /Cluster
    data/P2/output02/output``.csv", #], "Table",
    "HeaderLines" → 0, "FieldSeparators" → "\t", "NumberPoint" → ".",
    CharacterEncoding → "UTF8"]][All, Range[1, 11]][
  All, Rule @@@ Transpose[{ToString@StringForm["Band ``", #] & /@
    Range[1, 11] // Evaluate, Range[1, 11]}] //
  Association] & /@ {"MegaFineUp", "MegaFineDown"};

In[*]:= data = Table[Transpose[
  {Range[0.001, 1.0, 0.001], di[All, ToString@StringForm["Band ``", #]]} //
  Normal] & /@ Range[1, 11], {di, data}];

```

```

In[*]:= ListLinePlot[#, ImageSize -> Full,
  PlotStyle -> AbsoluteThickness[0.5], PlotRange -> {-7, 3}] & /@ data // TableForm

```

Out[*] // TableForm =

