```
(*CsPbBr3*)

h = 6.58 * 10^-16;

c = 3 * 10^14;

T = 2.309;

LT = 0.0063;

M = 0.214;

k[y_] := (y + T)/(c * h)

b = 4.96;

EB = 13.6 (*Hidrigen atm energy in eV *);
aB = 0.53 * 10^-4 (* in microns*);

κ[y_] := b (1 - LT/y)

γ-[x_, y_] := (x^2 - κ[y] * (k[y])^2)^1/2

(*Here I make the formula for the partial derivative of A*)

pA[x_, y_] := 1 + γ-[x, y]/(b * (x^2 - (k[y])^2)^1/2) +
  y ((-((b*LT)/y^2) * (k[y])^2 + κ[y] * (2 k[y])/(c*h))/(2 * b * γ-[x, y] * (x^2 - (k[y])^2)^1/2) +
    (γ-[x, y] * k[y])/(b * c * h (x^2 - (k[y])^2) * (x^2 - (k[y])^2)^1/2))

(*Here I make the formula for the real part of the correction term*)

R[x_, y_] :=
  (EB * aB^2)^1/2 * (LT * x^2)/(b * (M * (LT - y))^1/2 * (x^2 - (k[y])^2)^1/2) (*Real part of correction*)

(*Here I make the formula for the imaginary part of the correction term*)

H[x_, y_] := (-EB * (aB)^2 * y * x^2)/(M (y (LT - y))^1/2) (*Imaginary part of correction*)

(*Here I make the formula for the real part of the Delta term*)

DR[x_, y_] := -R[x, y] / pA[x, y] (*delta real*)

(*Here I make the formula for the imaginary part of the Delta term*)

DI[x_, y_] := -H[x, y] / pA[x, y] (*delta imaginary*)
```

```
(*partial of energy with respect to momentum for infinite mass dispersion*)
pE[x_, y_] := 2 * x / (2 k[y]/(c*h) * κ[y]/(κ[y]+1) + (k[y])^2*b*LT/(y^2 (κ[y]+1)^2))

df = D[-R[x, y] / pA[x, y], x];
(*partial of the energy correction with respect to momentum*)

d[xVal_, yVal_] := df /. {x → xVal, y → yVal} (*evaluating partial function*)

V[x_, y_] := pE[x, y] + d[x, y] (*velocity of surface exciton polariton*)

j[x_] := Solve[x^2 == (k[y])^2 * κ[y]/(κ[y] + 1), y]

middleSolution[x_] := y /. j[x][[2]]

qs1part1 = Range[11, 13, 0.1];

qs1part3 = Range[13, 15, 0.5];

qs1part2 = Range[15, 60, 0.75];

qs1 = Join[qs1part1, qs1part3, qs1part2]
```

Out[ ]=

```
{11., 11.1, 11.2, 11.3, 11.4, 11.5, 11.6, 11.7, 11.8, 11.9, 12., 12.1, 12.2,
 12.3, 12.4, 12.5, 12.6, 12.7, 12.8, 12.9, 13., 13., 13.5, 14., 14.5, 15., 15.,
 15.75, 16.5, 17.25, 18., 18.75, 19.5, 20.25, 21., 21.75, 22.5, 23.25, 24.,
 24.75, 25.5, 26.25, 27., 27.75, 28.5, 29.25, 30., 30.75, 31.5, 32.25, 33.,
 33.75, 34.5, 35.25, 36., 36.75, 37.5, 38.25, 39., 39.75, 40.5, 41.25, 42.,
 42.75, 43.5, 44.25, 45., 45.75, 46.5, 47.25, 48., 48.75, 49.5, 50.25, 51.,
 51.75, 52.5, 53.25, 54., 54.75, 55.5, 56.25, 57., 57.75, 58.5, 59.25, 60.}
```

```
qs1 = Append[qs1, 60];

yValues1 = middleSolution /@ qs1;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

General : Further output of Solve::ratnz will be suppressed during this calculation.

In[•]:=
```
xyPairs1 = Transpose[{qs1, yValues1}]
```

Out[•]=
```
{{11., -0.00954062}, {11.1, -0.0067152}, {11.2, -0.00471322},
 {11.3, -0.00324227}, {11.4, -0.00212534}, {11.5, -0.00125284},
 {11.6, -0.000554746}, {11.7, 0.0000152432}, {11.8, 0.000488712},
 {11.9, 0.000887831}, {12., 0.00122856}, {12.1, 0.00152267}, {12.2, 0.00177897},
 {12.3, 0.00200424}, {12.4, 0.00220372}, {12.5, 0.00238156}, {12.6, 0.00254105},
 {12.7, 0.00268487}, {12.8, 0.00281519}, {12.9, 0.00293381}, {13., 0.00304221},
 {13., 0.00304221}, {13.5, 0.00346875}, {14., 0.00376609}, {14.5, 0.00398476},
 {15., 0.00415202}, {15., 0.00415202}, {15.75, 0.00433981}, {16.5, 0.00447795},
 {17.25, 0.00458352}, {18., 0.0046666}, {18.75, 0.00473351}, {19.5, 0.00478844},
 {20.25, 0.00483424}, {21., 0.00487293}, {21.75, 0.00490599},
 {22.5, 0.00493452}, {23.25, 0.00495934}, {24., 0.00498111}, {24.75, 0.00500032},
 {25.5, 0.00501738}, {26.25, 0.00503261}, {27., 0.00504627}, {27.75, 0.00505859},
 {28.5, 0.00506973}, {29.25, 0.00507985}, {30., 0.00508908}, {30.75, 0.00509751},
 {31.5, 0.00510524}, {32.25, 0.00511235}, {33., 0.00511891}, {33.75, 0.00512497},
 {34.5, 0.00513058}, {35.25, 0.00513579}, {36., 0.00514064}, {36.75, 0.00514515},
 {37.5, 0.00514937}, {38.25, 0.00515331}, {39., 0.005157}, {39.75, 0.00516047},
 {40.5, 0.00516372}, {41.25, 0.00516678}, {42., 0.00516966}, {42.75, 0.00517238},
 {43.5, 0.00517495}, {44.25, 0.00517738}, {45., 0.00517967}, {45.75, 0.00518185},
 {46.5, 0.00518392}, {47.25, 0.00518588}, {48., 0.00518774}, {48.75, 0.00518951},
 {49.5, 0.00519119}, {50.25, 0.0051928}, {51., 0.00519433}, {51.75, 0.00519579},
 {52.5, 0.00519719}, {53.25, 0.00519852}, {54., 0.0051998}, {54.75, 0.00520102},
 {55.5, 0.00520219}, {56.25, 0.00520331}, {57., 0.00520438}, {57.75, 0.00520541},
 {58.5, 0.0052064}, {59.25, 0.00520735}, {60., 0.00520827}, {60, 0.00520827}}
```

```
In[ ]:= realcorrection1 = DR @@@ xyPairs1
```

```
Out[ ]=
{0. + 0.0000573746 i, 0. + 0.000065437 i, 0. + 0.0000731466 i, 0. + 0.0000799927 i,
 0. + 0.0000849677 i, 0. + 0.0000857602 i, 0. + 0.0000757816 i, -0.0000168695,
 -0.000095173, -0.000127763, -0.000149664, -0.000165918, -0.000178601,
 -0.000188819, -0.000197243, -0.000204315, -0.000210339, -0.000215537,
 -0.000220071, -0.000224066, -0.000227619, -0.000227619, -0.000240933,
 -0.000250061, -0.000257215, -0.000263385, -0.000263385, -0.000271792,
 -0.000279816, -0.000287776, -0.000295807, -0.000303963, -0.000312262,
 -0.000320704, -0.000329283, -0.000337989, -0.000346812, -0.00035574,
 -0.000364764, -0.000373875, -0.000383065, -0.000392327, -0.000401654,
 -0.00041104, -0.00042048, -0.00042997, -0.000439505, -0.000449081,
 -0.000458696, -0.000468346, -0.000478029, -0.000487742, -0.000497484,
 -0.000507251, -0.000517043, -0.000526857, -0.000536692, -0.000546548,
 -0.000556421, -0.000566313, -0.00057622, -0.000586143, -0.000596081,
 -0.000606032, -0.000615996, -0.000625972, -0.00063596, -0.000645959,
 -0.000655968, -0.000665987, -0.000676015, -0.000686052, -0.000696098,
 -0.000706151, -0.000716213, -0.000726281, -0.000736357, -0.000746439,
 -0.000756528, -0.000766623, -0.000776723, -0.00078683, -0.000796941,
 -0.000807058, -0.00081718, -0.000827306, -0.000837437, -0.000837437}
```

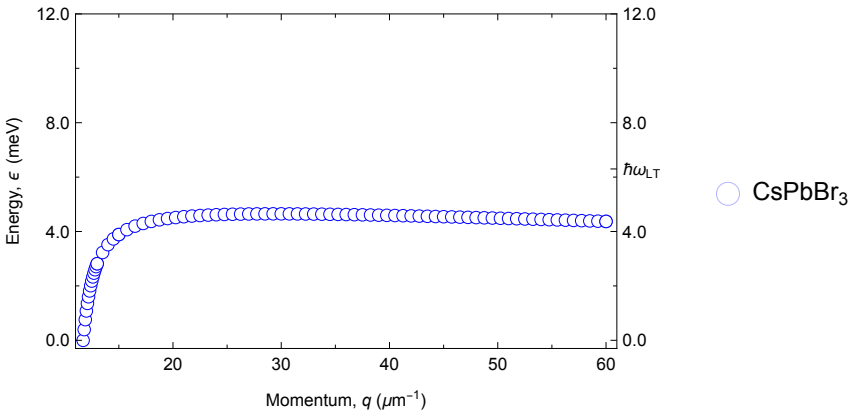
```
In[ ]:= actualReal1 = yValues1 + realcorrection1;
```

In[•]:=
```
group1 = Transpose[{qs1, actualReal1}]
```

Out[•]=
```
{{11., -0.00954062 + 0.0000573746 i}, {11.1, -0.0067152 + 0.000065437 i},
 {11.2, -0.00471322 + 0.0000731466 i}, {11.3, -0.00324227 + 0.0000799927 i},
 {11.4, -0.00212534 + 0.0000849677 i}, {11.5, -0.00125284 + 0.0000857602 i},
 {11.6, -0.000554746 + 0.0000757816 i}, {11.7, -1.62629 × 10^-6},
 {11.8, 0.000393539}, {11.9, 0.000760068}, {12., 0.0010789}, {12.1, 0.00135675},
 {12.2, 0.00160037}, {12.3, 0.00181542}, {12.4, 0.00200648}, {12.5, 0.00217724},
 {12.6, 0.00233071}, {12.7, 0.00246933}, {12.8, 0.00259512}, {12.9, 0.00270974},
 {13., 0.0028146}, {13., 0.0028146}, {13.5, 0.00322781}, {14., 0.00351603},
 {14.5, 0.00372755}, {15., 0.00388864}, {15., 0.00388864}, {15.75, 0.00406802},
 {16.5, 0.00419813}, {17.25, 0.00429574}, {18., 0.00437079}, {18.75, 0.00442955},
 {19.5, 0.00447618}, {20.25, 0.00451354}, {21., 0.00454365}, {21.75, 0.004568},
 {22.5, 0.00458771}, {23.25, 0.0046036}, {24., 0.00461634}, {24.75, 0.00462644},
 {25.5, 0.00463431}, {26.25, 0.00464028}, {27., 0.00464462}, {27.75, 0.00464755},
 {28.5, 0.00464925}, {29.25, 0.00464988}, {30., 0.00464957}, {30.75, 0.00464843},
 {31.5, 0.00464655}, {32.25, 0.00464401}, {33., 0.00464088}, {33.75, 0.00463723},
 {34.5, 0.0046331}, {35.25, 0.00462854}, {36., 0.0046236}, {36.75, 0.0046183},
 {37.5, 0.00461268}, {38.25, 0.00460676}, {39., 0.00460058}, {39.75, 0.00459415},
 {40.5, 0.0045875}, {41.25, 0.00458064}, {42., 0.00457358}, {42.75, 0.00456635},
 {43.5, 0.00455895}, {44.25, 0.00455141}, {45., 0.00454371}, {45.75, 0.00453589},
 {46.5, 0.00452795}, {47.25, 0.00451989}, {48., 0.00451172}, {48.75, 0.00450346},
 {49.5, 0.0044951}, {50.25, 0.00448665}, {51., 0.00447812}, {51.75, 0.00446951},
 {52.5, 0.00446083}, {53.25, 0.00445208}, {54., 0.00444327}, {54.75, 0.0044344},
 {55.5, 0.00442546}, {56.25, 0.00441648}, {57., 0.00440744}, {57.75, 0.00439836},
 {58.5, 0.00438922}, {59.25, 0.00438005}, {60., 0.00437083}, {60, 0.00437083}}
```

In[ ]:=
```
curr1 = yValues1 + Re[realcorrection1];
pair1 = Transpose[{qs1, curr1}];
s1 = ListPlot[pair1, PlotMarkers → {Graphics[{EdgeForm[Blue], White, Disk[]}], 7},
  FrameLabel → {{Row[{"Energy, ", Style["ϵ", Italic], " (meV)"}], ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1)"}], ""}}, Frame → True,
  FrameTicks → {{{{0, "0.0"}, {0.002, "", {0.003, 0}}, {0.004, "4.0"}, {0.006,
       "", {0.003, 0}}, {0.008, "8.0"}, {0.01, "", {0.003, 0}}, {0.012, "12.0"}},
     {{0, "0.0"}, {0.002, "", {0.003, 0}}, {0.004, "4.0"}, {0.006, "", {0.003, 0}},
      {0.008, "8.0"}, {0.01, "", {0.003, 0}}, {0.012, "12.0"}, {0.0063, "ħω_LT"}}},
    {{{10, "10"}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, "10"}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}},
      {30, ""}, {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.0003, 0.012}}, PlotLegends → {"CsPbBr3"}]
```

Out[ ]=



In[ ]:=
```
qs1 = Range[10.75, 60, 1];
yValues1 = middleSolution /@ qs1;
xyPairs1 = Transpose[{qs1, yValues1}];
realcorrection1 = DR @@@ xyPairs1;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

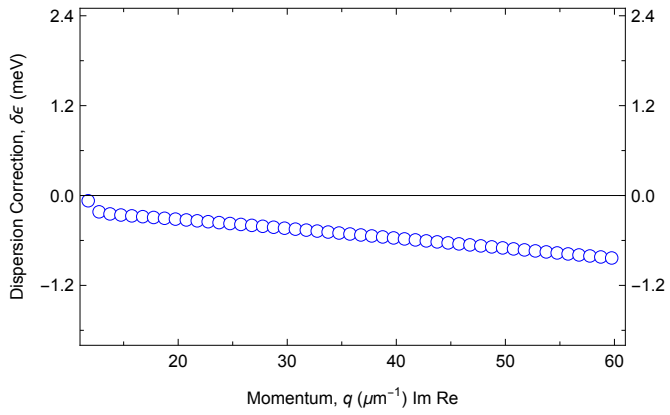
General : Further output of Solve::ratnz will be suppressed during this calculation.

In[ ]:=
```
imaginarycorrection1 = DI @@@ xyPairs1;
```

In[ ]:=
```
qandreal1 = Transpose[{qs1, realcorrection1}];
```

In[ ]:=
```
qversusreal1 =
 ListPlot[qandreal1, PlotMarkers → {Graphics[{EdgeForm[Blue], White, Disk[]}], 7},
  FrameLabel → {{"Dispersion Correction, δϵ (meV)", ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1) Im Re"}], ""}},
  Frame → True, FrameTicks → {{{{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"},
      {-0.0006, "", {0.003, 0}}, {0, "0.0"}, {0.0006, "", {0.003, 0}},
      {0.0012, "1.2"}, {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}},
     {{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"}, {-0.0006, "", {0.003, 0}},
      {0, "0.0"}, {0.0006, "", {0.003, 0}}, {0.0012, "1.2"},
      {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}}},
    {{{10, ""}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, ""}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}}, {30, ""},
      {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.002, 0.0025}}]
```

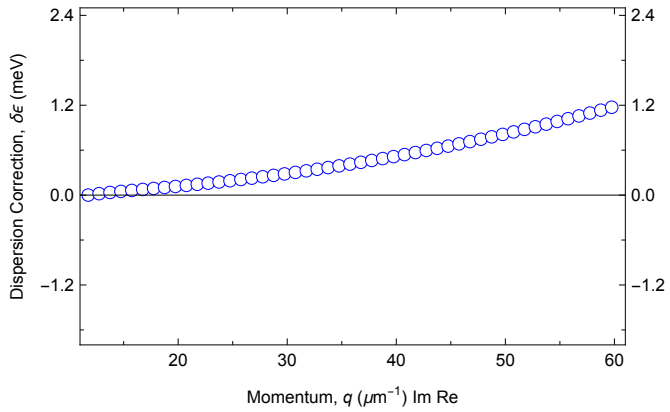
Out[ ]=



In[ ]:=
```
qandimaginary1 = Transpose[{qs1, imaginarycorrection1}];
```

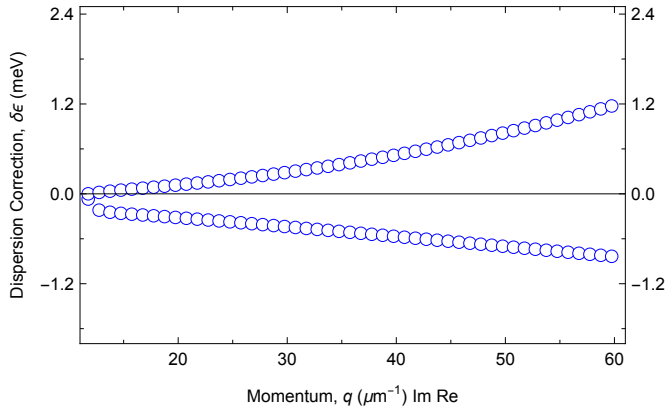
In[ ]:=
```
qversusimaginary1 = ListPlot[qandimaginary1,
  PlotMarkers → {Graphics[{EdgeForm[Blue], White, Disk[]}], 7},
  FrameLabel → {{"Dispersion Correction, δϵ (meV)", ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1) Im Re"}], ""}},
  Frame → True, FrameTicks → {{{{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"},
      {-0.0006, "", {0.003, 0}}, {0, "0.0"}, {0.0006, "", {0.003, 0}},
      {0.0012, "1.2"}, {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}},
     {{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"}, {-0.0006, "", {0.003, 0}},
      {0, "0.0"}, {0.0006, "", {0.003, 0}}, {0.0012, "1.2"},
      {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}}},
    {{{10, ""}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, ""}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}}, {30, ""},
      {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.002, 0.0025}}]
```

Out[ ]=



In[ ]:=
```
y1 = Show[qversusreal1, qversusimaginary1]
```

Out[ ]=



```
In[ ]:= frontV1 = Range[0.01, 8.9, 0.25];

In[ ]:= firstHalfV1 = Range[9, 10, 0.1];

In[ ]:= middleV1 = Range[10, 11, 0.02];

In[ ]:= thirdV1 = Range[11.1, 12, 0.1];

In[ ]:= secondHalfV1 = Range[12, 27, 0.15];

In[ ]:= qsV1 = Join[frontV1, firstHalfV1, middleV1, thirdV1, secondHalfV1];

In[ ]:= yValuesforV1 = middleSolution /@ qsV1;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

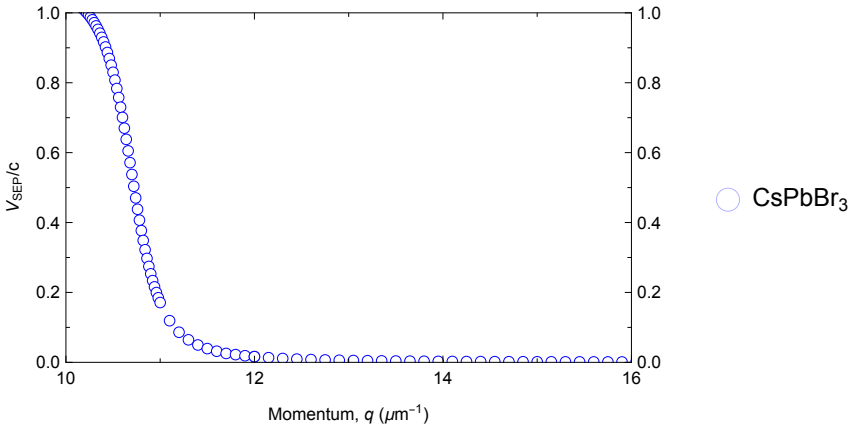
General : Further output of Solve::ratnz will be suppressed during this calculation.

```
In[ ]:= xyPairsForV1 = Transpose[{qsV1, yValuesforV1}];

In[ ]:= Velocities1 = V @@@ xyPairsForV1;

In[ ]:= VasFuncQ1 = Transpose[{qsV1, Re[Velocities1] / (c * h)}]

Out[ ]=
{{0.01, 1.09593}, {0.26, 1.09592}, {0.51, 1.09591}, {0.76, 1.09589}, {1.01, 1.09588},
 {1.26, 1.09586}, {1.51, 1.09584}, {1.76, 1.09582}, {2.01, 1.0958}, {2.26, 1.09578},
 {2.51, 1.09575}, {2.76, 1.09573}, {3.01, 1.0957}, {3.26, 1.09566},
 {3.51, 1.09563}, {3.76, 1.09559}, {4.01, 1.09554}, {4.26, 1.09549},
 {4.51, 1.09543}, {4.76, 1.09537}, {5.01, 1.0953}, {5.26, 1.09521},
 {5.51, 1.09512}, {5.76, 1.09501}, {6.01, 1.09488}, {6.26, 1.09473},
 {6.51, 1.09455}, {6.76, 1.09434}, {7.01, 1.09408}, {7.26, 1.09377},
 {7.51, 1.09338}, {7.76, 1.09288}, {8.01, 1.09225}, {8.26, 1.09141},
 {8.51, 1.09027}, {8.76, 1.08868}, {9., 1.08646}, {9.1, 1.08524}, {9.2, 1.08378},
 {9.3, 1.08201}, {9.4, 1.07983}, {9.5, 1.07713}, {9.6, 1.0737}, {9.7, 1.0693},
 {9.8, 1.0635}, {9.9, 1.0557}, {10., 1.04489}, {10., 1.04489}, {10.02, 1.04224},
 {10.04, 1.0394}, {10.06, 1.03633}, {10.08, 1.03303}, {10.1, 1.02946},
 {10.12, 1.0256}, {10.14, 1.02143}, {10.16, 1.0169}, {10.18, 1.01198},
 {10.2, 1.00664}, {10.22, 1.00082}, {10.24, 0.994478}, {10.26, 0.987553},
 {10.28, 0.979983}, {10.3, 0.971701}, {10.32, 0.962629}, {10.34, 0.952685},
 {10.36, 0.941778}, {10.38, 0.929811}, {10.4, 0.916681}, {10.42, 0.902281},
 {10.44, 0.886502}, {10.46, 0.869235}, {10.48, 0.850379}, {10.5, 0.829844},
 {10.52, 0.807559}, {10.54, 0.783484}, {10.56, 0.757615}, {10.58, 0.729996},
 {10.6, 0.700728}, {10.62, 0.669974}, {10.64, 0.63796}, {10.66, 0.604973},
 {10.68, 0.571349}, {10.7, 0.53746}, {10.72, 0.503691}, {10.74, 0.470424},
```

{10.76, 0.438008}, {10.78, 0.406752}, {10.8, 0.376905}, {10.82, 0.348653},
{10.84, 0.32212}, {10.86, 0.297371}, {10.88, 0.274419}, {10.9, 0.253235},
{10.92, 0.23376}, {10.94, 0.215909}, {10.96, 0.199585}, {10.98, 0.184681},
{11., 0.171088}, {11.1, 0.119154}, {11.2, 0.086087}, {11.3, 0.0644004},
{11.4, 0.0496671}, {11.5, 0.0393103}, {11.6, 0.0318022}, {11.7, 0.0254828},
{11.8, 0.02212}, {11.9, 0.0189012}, {12., 0.0163085}, {12., 0.0163085},
{12.15, 0.0132969}, {12.3, 0.0110374}, {12.45, 0.00930212}, {12.6, 0.0079418},
{12.75, 0.00685631}, {12.9, 0.00597661}, {13.05, 0.00525395}, {13.2, 0.00465314},
{13.35, 0.0041483}, {13.5, 0.00372005}, {13.65, 0.00335367}, {13.8, 0.00303779},
{13.95, 0.00276355}, {14.1, 0.00252394}, {14.25, 0.00231337}, {14.4, 0.00212733},
{14.55, 0.00196215}, {14.7, 0.00181482}, {14.85, 0.00168287}, {15., 0.00156422},
{15.15, 0.00145715}, {15.3, 0.0013602}, {15.45, 0.00127212}, {15.6, 0.00119188},
{15.75, 0.00111856}, {15.9, 0.0010514}, {16.05, 0.00098972}, {16.2, 0.000932943},
{16.35, 0.000880563}, {16.5, 0.000832138}, {16.65, 0.000787279},
{16.8, 0.000745645}, {16.95, 0.000706935}, {17.1, 0.000670882},
{17.25, 0.000637247}, {17.4, 0.000605821}, {17.55, 0.000576413},
{17.7, 0.000548855}, {17.85, 0.000522996}, {18., 0.000498698},
{18.15, 0.000475839}, {18.3, 0.000454308}, {18.45, 0.000434005},
{18.6, 0.000414837}, {18.75, 0.000396722}, {18.9, 0.000379585},
{19.05, 0.000363356}, {19.2, 0.000347973}, {19.35, 0.000333378},
{19.5, 0.000319519}, {19.65, 0.000306347}, {19.8, 0.000293818},
{19.95, 0.00028189}, {20.1, 0.000270526}, {20.25, 0.000259691},
{20.4, 0.000249354}, {20.55, 0.000239483}, {20.7, 0.000230052},
{20.85, 0.000221036}, {21., 0.000212409}, {21.15, 0.000204151},
{21.3, 0.00019624}, {21.45, 0.000188658}, {21.6, 0.000181387},
{21.75, 0.00017441}, {21.9, 0.000167712}, {22.05, 0.000161278},
{22.2, 0.000155094}, {22.35, 0.000149148}, {22.5, 0.000143428},
{22.65, 0.000137922}, {22.8, 0.00013262}, {22.95, 0.000127513},
{23.1, 0.000122591}, {23.25, 0.000117845}, {23.4, 0.000113267},
{23.55, 0.000108849}, {23.7, 0.000104584}, {23.85, 0.000100465},
{24., 0.0000964857}, {24.15, 0.0000926395}, {24.3, 0.0000889209},
{24.45, 0.0000853243}, {24.6, 0.0000818444}, {24.75, 0.0000784763},
{24.9, 0.0000752154}, {25.05, 0.0000720572}, {25.2, 0.0000689975},
{25.35, 0.0000660322}, {25.5, 0.0000631576}, {25.65, 0.0000603701},
{25.8, 0.0000576662}, {25.95, 0.0000550427}, {26.1, 0.0000524964},
{26.25, 0.0000500244}, {26.4, 0.0000476239}, {26.55, 0.0000452921},
{26.7, 0.0000430266}, {26.85, 0.0000408247}, {27., 0.0000386844}}

In[ ]:=
```
v1 = ListPlot[VasFuncQ1,
  PlotMarkers → {Graphics[{EdgeForm[Blue], White, Disk[]}], 6}, FrameLabel →
   {{"V_SEP/c", ""}, {Row[{"Momentum, ", Style["q", Italic], " (μm^-1)"}], ""}},
  Frame → True, FrameTicks → {{{{0.0, "0.0"}, {0.1, "", {0.003, 0}}, {0.2, "0.2"},
      {0.3, "", {0.003, 0}}, {0.4, "0.4"}, {0.5, "", {0.003, 0}}, {0.6, "0.6"},
      {0.7, "", {0.003, 0}}, {0.8, "0.8"}, {0.9, "", {0.003, 0}}, {1.0, "1.0"}},
     {{0.0, "0.0"}, {0.1, "", {0.003, 0}}, {0.2, "0.2"}, {0.3, "", {0.003, 0}},
      {0.4, "0.4"}, {0.5, "", {0.003, 0}}, {0.6, "0.6"}, {0.7, "", {0.003, 0}},
      {0.8, "0.8"}, {0.9, "", {0.003, 0}}, {1.0, "1.0"}}},
    {{{8, "8"}, {9, "", {0.003, 0}}, {10, "10"}, {11, "", {0.003, 0}},
      {12, "12"}, {13, "", {0.003, 0}}, {14, "14"}, {15, "", {0.003, 0}},
      {16, "16"}, {17, "", {0.003, 0}}, {18, "18"}}, {{8, ""}, {9, "", {0.003, 0}},
      {10, ""}, {11, "", {0.003, 0}}, {12, ""}, {13, "", {0.003, 0}}, {14, ""},
      {15, "", {0.003, 0}}, {16, ""}, {17, "", {0.003, 0}}, {18, ""}}}},
  PlotLegends → {"CsPbBr3"}, PlotRange → {{10, 16}, {0, 1}}]
```

Out[ ]=



In[ ]:=
```
(*CsPbCl3*)
```

```
In[ ]:= T = 2.992;
        LT = 0.0107;
        M = 0.283;
        k[y_] := (y + T)/(c * h)
        b = 4.07;
        κ[y_] := b (1 - LT/y)
        γ-[x_, y_] := (x^2 - κ[y] * (k[y])^2)^1/2
        pA[x_, y_] := 1 + γ-[x, y]/(b * (x^2 - (k[y])^2)^1/2) +
          y ((-(b*LT/y^2 * (k[y])^2 + κ[y] * 2 k[y]/(c*h)))/(2 * b * γ-[x, y] * (x^2 - (k[y])^2)^1/2) + γ-[x, y] * k[y]/(b * c * h (x^2 - (k[y])^2) * (x^2 - (k[y])^2)^1/2))
        R[x_, y_] := (EB * aB^2)^1/2 * LT * x^2/(b * (M * (LT - y))^1/2 * (x^2 - (k[y])^2)^1/2)
        (*Real part of correction*)

        H[x_, y_] := -EB * (aB)^2 * y * x^2/(M (y (LT - y))^1/2) (*Imaginary part of correction*)

        DR[x_, y_] := -R[x, y] / pA[x, y] (*delta real*)

        DI[x_, y_] := -H[x, y] / pA[x, y] (*delta imaginary*)

        pE[x_, y_] := 2 * x/(2 k[y]/(c*h) * κ[y]/(κ[y]+1) + (k[y])^2*b*LT/(y^2 (κ[y]+1)^2))
        df = D[-R[x, y] / pA[x, y], x];
        d[xVal_, yVal_] := df /. {x → xVal, y → yVal}
        V[x_, y_] := pE[x, y] + d[x, y]
        j[x_] := Solve[x^2 == (k[y])^2 * κ[y]/(κ[y] + 1), y]
        middleSolution[x_] := y /. j[x][[2]]
In[ ]:= qs2part1 = Range[13, 18, 0.10];
In[ ]:= qs2part2 = Range[18, 60, 0.75];
In[ ]:=
In[ ]:= qs2 = Join[qs2part1, qs2part2];
In[ ]:=
```

```
In[ ]:= qs2 = Append[qs2, 60];

In[ ]:= yValues2 = middleSolution /@ qs2;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

General : Further output of Solve::ratnz will be suppressed during this calculation.

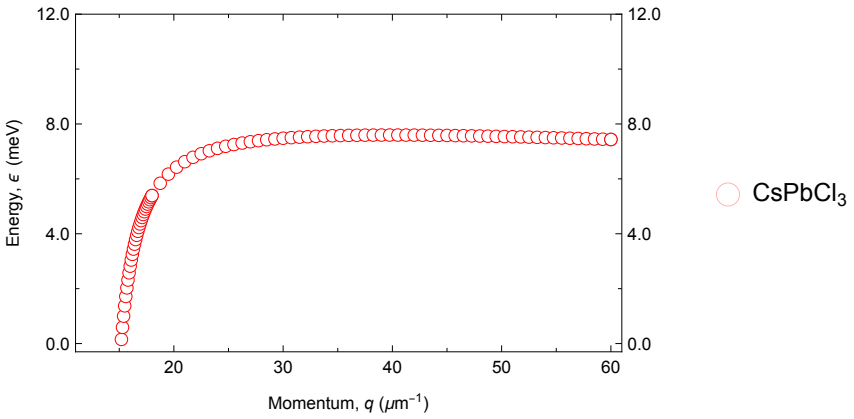
```
In[ ]:= xyPairs2 = Transpose[{qs2, yValues2}];

In[ ]:= realcorrection2 = DR @@@ xyPairs2;

In[ ]:= actualReal2 = yValues2 + realcorrection2

Out[ ]=
{-0.147062 + 0.0000292625 i, -0.127871 + 0.0000319441 i, -0.109434 + 0.0000351072 i,
 -0.0920063 + 0.0000388654 i, -0.0759054 + 0.0000433404 i, -0.0614833 + 0.0000486373 i,
 -0.0490455 + 0.0000548021 i, -0.0387407 + 0.0000617864 i, -0.0304931 + 0.0000694474 i,
 -0.0240377 + 0.0000775926 i, -0.0190268 + 0.00008603 i, -0.0151254 + 0.0000945916 i,
 -0.0120565 + 0.000103128 i, -0.00960939 + 0.000111486 i, -0.00762889 + 0.000119476 i,
 -0.00600258 + 0.000126833 i, -0.00464874 + 0.000133151 i, -0.00350753 + 0.000137766 i,
 -0.00253459 + 0.000139539 i, -0.0016966 + 0.000136334 i, -0.000968207 + 0.000123534 i,
 -0.000329831 + 0.0000870936 i, 0.000151891, 0.000590042, 0.000999765,
 0.00137444, 0.00171631, 0.00202867, 0.00231477, 0.00257757, 0.00281964,
 0.00304325, 0.00325035, 0.00344264, 0.00362163, 0.0037886, 0.00394469,
 0.00409092, 0.00422815, 0.00435719, 0.00447872, 0.00459337, 0.00470168,
 0.00480416, 0.00490126, 0.00499336, 0.00508085, 0.00516405, 0.00524325,
 0.00531874, 0.00539075, 0.00539075, 0.00584016, 0.00617229, 0.00642631,
 0.00662573, 0.00678551, 0.00691561, 0.00702294, 0.00711241, 0.00718763,
 0.0072513, 0.00730549, 0.0073518, 0.0073915, 0.0074256, 0.00745492,
 0.00748012, 0.00750175, 0.00752028, 0.00753608, 0.00754948, 0.00756076,
 0.00757016, 0.00757787, 0.00758407, 0.00758891, 0.00759253, 0.00759504,
 0.00759654, 0.00759714, 0.0075969, 0.00759589, 0.00759419, 0.00759185,
 0.00758891, 0.00758543, 0.00758145, 0.007577, 0.00757212, 0.00756684,
 0.00756119, 0.00755519, 0.00754886, 0.00754223, 0.00753532, 0.00752815,
 0.00752073, 0.00751307, 0.0075052, 0.00749712, 0.00748884, 0.00748039,
 0.00747176, 0.00746297, 0.00745402, 0.00744493, 0.0074357, 0.0074357}
```

In[ ]:=
```
group2 = Transpose[{qs2, actualReal2}]
```

Out[ ]=
```
{{13., -0.147062 + 0.0000292625 i}, {13.1, -0.127871 + 0.0000319441 i},
 {13.2, -0.109434 + 0.0000351072 i}, {13.3, -0.0920063 + 0.0000388654 i},
 {13.4, -0.0759054 + 0.0000433404 i}, {13.5, -0.0614833 + 0.0000486373 i},
 {13.6, -0.0490455 + 0.0000548021 i}, {13.7, -0.0387407 + 0.0000617864 i},
 {13.8, -0.0304931 + 0.0000694474 i}, {13.9, -0.0240377 + 0.0000775926 i},
 {14., -0.0190268 + 0.00008603 i}, {14.1, -0.0151254 + 0.0000945916 i},
 {14.2, -0.0120565 + 0.000103128 i}, {14.3, -0.00960939 + 0.000111486 i},
 {14.4, -0.00762889 + 0.000119476 i}, {14.5, -0.00600258 + 0.000126833 i},
 {14.6, -0.00464874 + 0.000133151 i}, {14.7, -0.00350753 + 0.000137766 i},
 {14.8, -0.00253459 + 0.000139539 i}, {14.9, -0.0016966 + 0.000136334 i},
 {15., -0.000968207 + 0.000123534 i}, {15.1, -0.000329831 + 0.0000870936 i},
 {15.2, 0.000151891}, {15.3, 0.000590042}, {15.4, 0.000999765},
 {15.5, 0.00137444}, {15.6, 0.00171631}, {15.7, 0.00202867}, {15.8, 0.00231477},
 {15.9, 0.00257757}, {16., 0.00281964}, {16.1, 0.00304325}, {16.2, 0.00325035},
 {16.3, 0.00344264}, {16.4, 0.00362163}, {16.5, 0.0037886}, {16.6, 0.00394469},
 {16.7, 0.00409092}, {16.8, 0.00422815}, {16.9, 0.00435719}, {17., 0.00447872},
 {17.1, 0.00459337}, {17.2, 0.00470168}, {17.3, 0.00480416}, {17.4, 0.00490126},
 {17.5, 0.00499336}, {17.6, 0.00508085}, {17.7, 0.00516405}, {17.8, 0.00524325},
 {17.9, 0.00531874}, {18., 0.00539075}, {18., 0.00539075}, {18.75, 0.00584016},
 {19.5, 0.00617229}, {20.25, 0.00642631}, {21., 0.00662573}, {21.75, 0.00678551},
 {22.5, 0.00691561}, {23.25, 0.00702294}, {24., 0.00711241}, {24.75, 0.00718763},
 {25.5, 0.0072513}, {26.25, 0.00730549}, {27., 0.0073518}, {27.75, 0.0073915},
 {28.5, 0.0074256}, {29.25, 0.00745492}, {30., 0.00748012}, {30.75, 0.00750175},
 {31.5, 0.00752028}, {32.25, 0.00753608}, {33., 0.00754948}, {33.75, 0.00756076},
 {34.5, 0.00757016}, {35.25, 0.00757787}, {36., 0.00758407}, {36.75, 0.00758891},
 {37.5, 0.00759253}, {38.25, 0.00759504}, {39., 0.00759654}, {39.75, 0.00759714},
 {40.5, 0.0075969}, {41.25, 0.00759589}, {42., 0.00759419}, {42.75, 0.00759185},
 {43.5, 0.00758891}, {44.25, 0.00758543}, {45., 0.00758145}, {45.75, 0.007577},
 {46.5, 0.00757212}, {47.25, 0.00756684}, {48., 0.00756119}, {48.75, 0.00755519},
 {49.5, 0.00754886}, {50.25, 0.00754223}, {51., 0.00753532}, {51.75, 0.00752815},
 {52.5, 0.00752073}, {53.25, 0.00751307}, {54., 0.0075052}, {54.75, 0.00749712},
 {55.5, 0.00748884}, {56.25, 0.00748039}, {57., 0.00747176}, {57.75, 0.00746297},
 {58.5, 0.00745402}, {59.25, 0.00744493}, {60., 0.0074357}, {60, 0.0074357}}
```

In[ ]:=
```
curr2 = yValues2 + realcorrection2;
pair2 = Transpose[{qs2, curr2}];
s2 = ListPlot[pair2, PlotMarkers → {Graphics[{EdgeForm[Red], White, Disk[]}], 7},
  FrameLabel → {{Row[{"Energy, ", Style["ϵ", Italic], " (meV)"}], ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1)"}], ""}} , Frame → True,
  FrameTicks → {{{{0, "0.0"}, {0.002, "", {0.003, 0}}, {0.004, "4.0"}, {0.006,
       "", {0.003, 0}}, {0.008, "8.0"}, {0.01, "", {0.003, 0}}, {0.012, "12.0"}},
     {{0, "0.0"}, {0.002, "", {0.003, 0}}, {0.004, "4.0"}, {0.006, "", {0.003, 0}},
      {0.008, "8.0"}, {0.01, "", {0.003, 0}}, {0.012, "12.0"}}},
    {{{10, "10"}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, "10"}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}},
      {30, ""}, {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.0003, 0.012}}, PlotLegends → {"CsPbCl₃"}]
```

Out[ ]=



In[ ]:=
```
qs2 = Range[10, 60, 0.75];
yValues2 = middleSolution /@ qs2;
xyPairs2 = Transpose[{qs2, yValues2}];
realcorrection2 = DR @@@ xyPairs2;
```

••• Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

••• Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

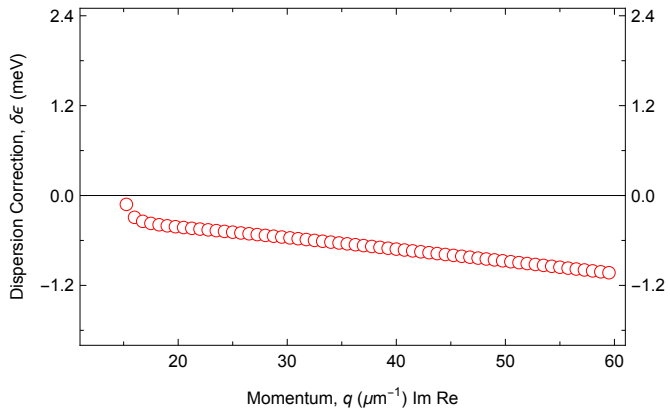
••• Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

••• General : Further output of Solve::ratnz will be suppressed during this calculation.

In[ ]:=
```
imaginarycorrection2 = DI @@@ xyPairs2;
```

```
In[•]:= qandreal2 = Transpose[{qs2, realcorrection2}];

In[•]:= qversusreal2 =
 ListPlot[qandreal2, PlotMarkers → {Graphics[{EdgeForm[Red], White, Disk[]}], 7},
  FrameLabel → {{"Dispersion Correction, δϵ (meV)", ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1) Im Re"}], ""}},
  Frame → True, FrameTicks → {{{{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"},
      {-0.0006, "", {0.003, 0}}, {0, "0.0"}, {0.0006, "", {0.003, 0}},
      {0.0012, "1.2"}, {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}},
     {{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"}, {-0.0006, "", {0.003, 0}},
      {0, "0.0"}, {0.0006, "", {0.003, 0}}, {0.0012, "1.2"},
      {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}}},
    {{{10, ""}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, ""}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}}, {30, ""},
      {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.002, 0.0025}}]
```

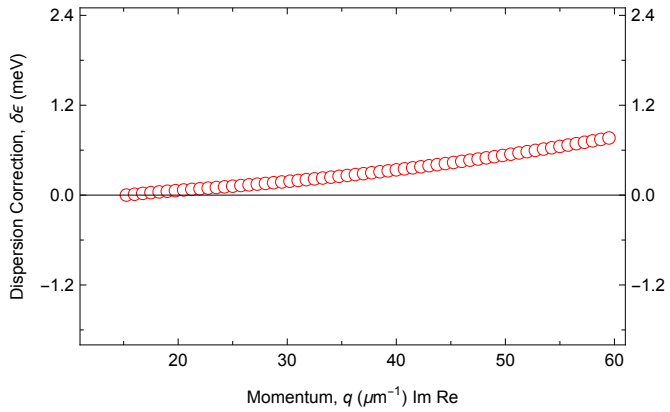
Out[•]=




```
In[•]:= qandimaginary2 = Transpose[{qs2, imaginarycorrection2}];
```

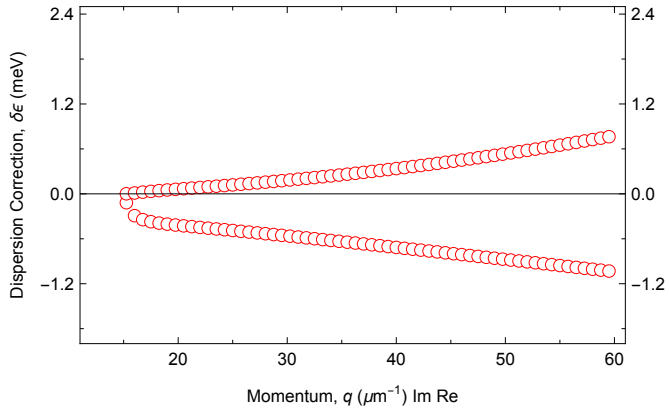
In[ ]:=
```
qversusimaginary2 = ListPlot[qandimaginary2,
  PlotMarkers → {Graphics[{EdgeForm[Red], White, Disk[]}], 7},
  FrameLabel → {{"Dispersion Correction, δϵ (meV)", ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1) Im Re"}], ""}},
  Frame → True, FrameTicks → {{{{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"},
      {-0.0006, "", {0.003, 0}}, {0, "0.0"}, {0.0006, "", {0.003, 0}},
      {0.0012, "1.2"}, {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}},
     {{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"}, {-0.0006, "", {0.003, 0}},
      {0, "0.0"}, {0.0006, "", {0.003, 0}}, {0.0012, "1.2"},
      {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}}},
    {{{10, ""}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, ""}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}}, {30, ""},
      {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.002, 0.0025}}]
```

Out[ ]=



In[ ]:=
```
y2 = Show[qversusreal2, qversusimaginary2]
```

Out[ ]=



In[ ]:=

In[ ]:=
```
frontV2 = Range[0.01, 10, 0.25];
```

In[ ]:=
```
firstHalfV2 = Range[10, 13, 0.1];
```

In[ ]:=
```
middleV2 = Range[13, 14, 0.02];
```

In[ ]:=
```
thirdV2 = Range[14, 17, 0.1];
```

In[ ]:=
```
secondHalfV2 = Range[17, 27, 0.15];
```

In[ ]:=
```
qsV2 = Join[frontV2, firstHalfV2, middleV2, thirdV2, secondHalfV2];
```

In[ ]:=
```
yValuesforV2 = middleSolution /@ qsV2;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

General : Further output of Solve::ratnz will be suppressed during this calculation.

In[ ]:=
```
xyPairsForV2 = Transpose[{qsV2, yValuesforV2}];
```

In[ ]:=
```
Velocities2 = V @@@ xyPairsForV2;
```

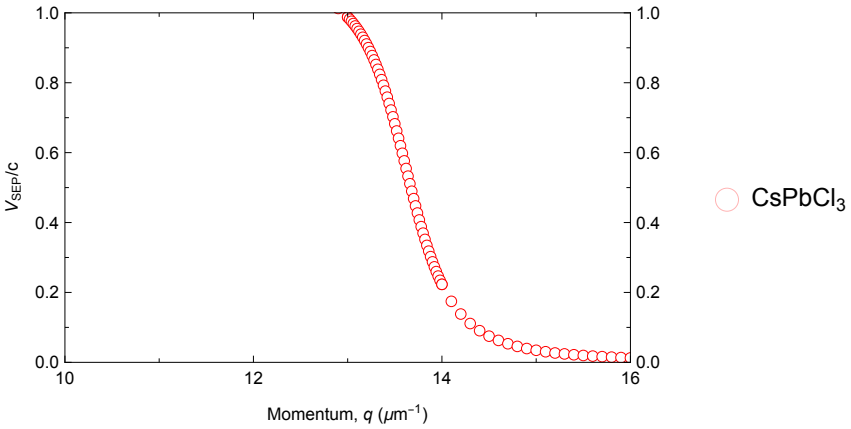
In[ ]:=
```
VasFuncQ2 = Transpose[{qsV2, Re[Velocities2] / (c * h)}]
```

Out[ ]=
```
{{0.01, 1.11572}, {0.26, 1.1157}, {0.51, 1.11569}, {0.76, 1.11567}, {1.01, 1.11565},
 {1.26, 1.11563}, {1.51, 1.11561}, {1.76, 1.11559}, {2.01, 1.11557},
 {2.26, 1.11555}, {2.51, 1.11552}, {2.76, 1.11549}, {3.01, 1.11546},
 {3.26, 1.11543}, {3.51, 1.1154}, {3.76, 1.11536}, {4.01, 1.11532}, {4.26, 1.11528},
 {4.51, 1.11523}, {4.76, 1.11518}, {5.01, 1.11513}, {5.26, 1.11507}, {5.51, 1.115},
 {5.76, 1.11493}, {6.01, 1.11486}, {6.26, 1.11477}, {6.51, 1.11467},
 {6.76, 1.11457}, {7.01, 1.11445}, {7.26, 1.11432}, {7.51, 1.11417}, {7.76, 1.114},
 {8.01, 1.11381}, {8.26, 1.11359}, {8.51, 1.11334}, {8.76, 1.11305},
 {9.01, 1.11271}, {9.26, 1.11231}, {9.51, 1.11184}, {9.76, 1.11128}, {10., 1.11063},
 {10.1, 1.11031}, {10.2, 1.10998}, {10.3, 1.10961}, {10.4, 1.1092}, {10.5, 1.10876},
 {10.6, 1.10828}, {10.7, 1.10774}, {10.8, 1.10715}, {10.9, 1.1065}, {11., 1.10577},
 {11.1, 1.10496}, {11.2, 1.10405}, {11.3, 1.10302}, {11.4, 1.10186},
 {11.5, 1.10054}, {11.6, 1.09903}, {11.7, 1.09729}, {11.8, 1.09528}, {11.9, 1.09293},
 {12., 1.09018}, {12.1, 1.08692}, {12.2, 1.08303}, {12.3, 1.07833}, {12.4, 1.0726},
 {12.5, 1.06554}, {12.6, 1.05672}, {12.7, 1.04554}, {12.8, 1.0312}, {12.9, 1.01251},
 {13., 0.98785}, {13., 0.98785}, {13.02, 0.982014}, {13.04, 0.975828},
 {13.06, 0.969271}, {13.08, 0.96232}, {13.1, 0.954948}, {13.12, 0.94713},
 {13.14, 0.93884}, {13.16, 0.93005}, {13.18, 0.920731}, {13.2, 0.910856},
 {13.22, 0.900396}, {13.24, 0.889324}, {13.26, 0.877614}, {13.28, 0.865239},
```

{13.3, 0.852179}, {13.32, 0.838413}, {13.34, 0.823927}, {13.36, 0.808711},
{13.38, 0.792761}, {13.4, 0.776081}, {13.42, 0.758681}, {13.44, 0.740582},
{13.46, 0.721814}, {13.48, 0.702419}, {13.5, 0.682446}, {13.52, 0.661957},
{13.54, 0.641023}, {13.56, 0.619725}, {13.58, 0.598151}, {13.6, 0.576394},
{13.62, 0.554553}, {13.64, 0.532728}, {13.66, 0.511018}, {13.68, 0.489521},
{13.7, 0.468329}, {13.72, 0.447528}, {13.74, 0.427195}, {13.76, 0.407399},
{13.78, 0.388197}, {13.8, 0.369637}, {13.82, 0.351756}, {13.84, 0.334582},
{13.86, 0.318131}, {13.88, 0.302413}, {13.9, 0.287429}, {13.92, 0.273172},
{13.94, 0.259631}, {13.96, 0.24679}, {13.98, 0.234628}, {14., 0.223122},
{14., 0.223122}, {14.1, 0.174502}, {14.2, 0.138193}, {14.3, 0.111042},
{14.4, 0.0905557}, {14.5, 0.0749003}, {14.6, 0.0627668}, {14.7, 0.0532282},
{14.8, 0.045626}, {14.9, 0.0394886}, {15., 0.0344743}, {15.1, 0.0303323},
{15.2, 0.0267659}, {15.3, 0.0240952}, {15.4, 0.0217093}, {15.5, 0.0196374},
{15.6, 0.017837}, {15.7, 0.0162663}, {15.8, 0.0148894}, {15.9, 0.0136766},
{16., 0.0126034}, {16.1, 0.0116495}, {16.2, 0.0107981}, {16.3, 0.0100351},
{16.4, 0.00934896}, {16.5, 0.00872965}, {16.6, 0.00816888}, {16.7, 0.00765953},
{16.8, 0.00719555}, {16.9, 0.00677174}, {17., 0.00638361}, {17., 0.00638361},
{17.15, 0.00585997}, {17.3, 0.005397}, {17.45, 0.0049857}, {17.6, 0.00461868},
{17.75, 0.00428983}, {17.9, 0.00399404}, {18.05, 0.00372705}, {18.2, 0.00348522},
{18.35, 0.00326552}, {18.5, 0.00306532}, {18.65, 0.00288238}, {18.8, 0.00271478},
{18.95, 0.00256086}, {19.1, 0.00241917}, {19.25, 0.00228844}, {19.4, 0.00216758},
{19.55, 0.00205563}, {19.7, 0.00195172}, {19.85, 0.00185511}, {20., 0.00176513},
{20.15, 0.00168119}, {20.3, 0.00160275}, {20.45, 0.00152936}, {20.6, 0.00146059},
{20.75, 0.00139606}, {20.9, 0.00133542}, {21.05, 0.00127838}, {21.2, 0.00122465},
{21.35, 0.00117398}, {21.5, 0.00112615}, {21.65, 0.00108094}, {21.8, 0.00103818},
{21.95, 0.000997684}, {22.1, 0.000959298}, {22.25, 0.000922879},
{22.4, 0.000888294}, {22.55, 0.000855425}, {22.7, 0.000824158},
{22.85, 0.000794393}, {23., 0.000766034}, {23.15, 0.000738996},
{23.3, 0.000713197}, {23.45, 0.000688564}, {23.6, 0.000665026},
{23.75, 0.000642522}, {23.9, 0.000620991}, {24.05, 0.000600379},
{24.2, 0.000580633}, {24.35, 0.000561707}, {24.5, 0.000543556},
{24.65, 0.000526139}, {24.8, 0.000509416}, {24.95, 0.000493351},
{25.1, 0.000477912}, {25.25, 0.000463065}, {25.4, 0.000448781},
{25.55, 0.000435032}, {25.7, 0.000421792}, {25.85, 0.000409036},
{26., 0.000396741}, {26.15, 0.000384886}, {26.3, 0.00037345}, {26.45, 0.000362413},
{26.6, 0.000351757}, {26.75, 0.000341465}, {26.9, 0.000331521}}

```
In[•]:= v2 = ListPlot[VasFuncQ2,
  PlotMarkers → {Graphics[{EdgeForm[Red], White, Disk[]}], 6}, FrameLabel →
   {{"V_SEP/c", ""}, {Row[{"Momentum, ", Style["q", Italic], " (μm^-1)"}], ""}},
  Frame → True, FrameTicks → {{{{0.0, "0.0"}, {0.1, "", {0.003, 0}}, {0.2, "0.2"},
      {0.3, "", {0.003, 0}}, {0.4, "0.4"}, {0.5, "", {0.003, 0}}, {0.6, "0.6"},
      {0.7, "", {0.003, 0}}, {0.8, "0.8"}, {0.9, "", {0.003, 0}}, {1.0, "1.0"}},
     {{0.0, "0.0"}, {0.1, "", {0.003, 0}}, {0.2, "0.2"}, {0.3, "", {0.003, 0}},
      {0.4, "0.4"}, {0.5, "", {0.003, 0}}, {0.6, "0.6"}, {0.7, "", {0.003, 0}},
      {0.8, "0.8"}, {0.9, "", {0.003, 0}}, {1.0, "1.0"}}},
    {{{8, "8"}, {9, "", {0.003, 0}}, {10, "10"}, {11, "", {0.003, 0}},
      {12, "12"}, {13, "", {0.003, 0}}, {14, "14"}, {15, "", {0.003, 0}},
      {16, "16"}, {17, "", {0.003, 0}}, {18, "18"}}, {{8, ""}, {9, "", {0.003, 0}},
      {10, ""}, {11, "", {0.003, 0}}, {12, ""}, {13, "", {0.003, 0}}, {14, ""},
      {15, "", {0.003, 0}}, {16, ""}, {17, "", {0.003, 0}}, {18, ""}}}},
  PlotLegends → {"CsPbCl3"}, PlotRange → {{10, 16}, {0, 1}}]
```

Out[•]=




```
In[•]:= T = (2.992 + 2.309) / 2;

In[•]:= LT = (0.0107 + 0.0063) / 2;

In[•]:= M = (0.283 + 0.214) / 2;

In[•]:= k[y_] := (y + T) / (c * h)

In[•]:= b = (4.07 + 4.96) / 2;

In[•]:= κ[y_] := b (1 - LT / y)

In[•]:= γ_[x_, y_] := (x^2 - κ[y] * (k[y])^2)^1/2
```

In[•]:=
$$pA[x\_, y\_] := 1 + \frac{\gamma_-[x, y]}{b * \left(x^2 - (k[y])^2\right)^{1/2}} + y\left(\frac{-\left(\frac{b*LT}{y^2} * (k[y])^2 + \varkappa[y] * \frac{2\,k[y]}{c*h}\right)}{2 * b * \gamma_-[x, y] * \left(x^2 - (k[y])^2\right)^{1/2}} + \frac{\gamma_-[x, y] * k[y]}{b * c * h\left(x^2 - (k[y])^2\right) * \left(x^2 - (k[y])^2\right)^{1/2}}\right)$$

In[•]:=
$$R[x\_, y\_] := \left(EB * aB^2\right)^{1/2} * \frac{LT * x^2}{b * (M * (LT - y))^{1/2} * \left(x^2 - (k[y])^2\right)^{1/2}}$$

```
(*Real part of correction*)

H[x_, y_] := -EB * (aB)^2 * y * x^2 / (M (y (LT - y))^(1/2)) (*Imaginary part of correction*)

DR[x_, y_] := -R[x, y] / pA[x, y] (*delta real*)

DI[x_, y_] := -H[x, y] / pA[x, y] (*delta imaginary*)

pE[x_, y_] := 2 * x / ((2 k[y])/(c*h) * κ[y]/(κ[y]+1) + (k[y])^2*b*LT/(y^2 (κ[y]+1)^2))
df = D[-R[x, y] / pA[x, y], x];
d[xVal_, yVal_] := df /. {x → xVal, y → yVal}
```

In[•]:=
```
V[x_, y_] := pE[x, y] + d[x, y]
```
In[•]:=
```
j[x_] := Solve[x^2 == (k[y])^2 * κ[y]/(κ[y] + 1), y]
middleSolution[x_] := y /. j[x][[2]]
```
In[•]:=
```
qs3part1 = Range[12.95, 14.7, 0.10];
```
In[•]:=
```
qs3part3 = Range[14.7, 16.4, 0.35];
```
In[•]:=
```
qs3part2 = Range[16.5, 60, 0.75];
```
In[•]:=

In[•]:=
```
qs3 = Join[qs3part1, qs3part3, qs3part2];
```
In[•]:=
```
qs3 = Append[qs3, 60];
```

```
In[•]:= yValues3 = middleSolution /@ qs3;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

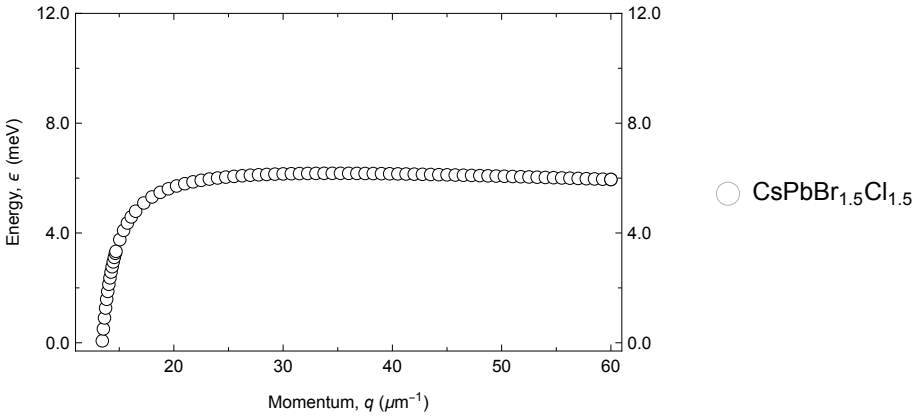
General : Further output of Solve::ratnz will be suppressed during this calculation.

```
In[•]:= xyPairs3 = Transpose[{qs3, yValues3}];

In[•]:= realcorrection3 = DR @@@ xyPairs3;

In[•]:= actualReal3 = yValues3 + realcorrection3;

In[•]:= group3 = Transpose[{qs3, actualReal3}]
```

```
Out[•]= {{12.95, -0.0040716 + 0.000104888 i}, {13.05, -0.00289757 + 0.000109886 i},
 {13.15, -0.00193438 + 0.000111584 i}, {13.25, -0.00113183 + 0.000106563 i},
 {13.35, -0.000454004 + 0.0000850323 i}, {13.45, 0.0000714722},
 {13.55, 0.000505766}, {13.65, 0.000906227}, {13.75, 0.00126437},
 {13.85, 0.00158449}, {13.95, 0.00187158}, {14.05, 0.00213013},
 {14.15, 0.00236399}, {14.25, 0.0025764}, {14.35, 0.00277011}, {14.45, 0.0029474},
 {14.55, 0.00311024}, {14.65, 0.00326028}, {14.7, 0.00333095},
 {15.05, 0.00375805}, {15.4, 0.00409342}, {15.75, 0.00436323}, {16.1, 0.00458461},
 {16.5, 0.00479309}, {17.25, 0.00509317}, {18., 0.00531292}, {18.75, 0.00547952},
 {19.5, 0.00560916}, {20.25, 0.00571207}, {21., 0.00579503}, {21.75, 0.00586273},
 {22.5, 0.00591849}, {23.25, 0.00596474}, {24., 0.00600331}, {24.75, 0.00603558},
 {25.5, 0.00606263}, {26.25, 0.0060853}, {27., 0.00610426}, {27.75, 0.00612007},
 {28.5, 0.00613316}, {29.25, 0.0061439}, {30., 0.0061526}, {30.75, 0.00615951},
 {31.5, 0.00616485}, {32.25, 0.0061688}, {33., 0.00617151}, {33.75, 0.00617312},
 {34.5, 0.00617374}, {35.25, 0.00617348}, {36., 0.00617242}, {36.75, 0.00617064},
 {37.5, 0.0061682}, {38.25, 0.00616517}, {39., 0.0061616}, {39.75, 0.00615753},
 {40.5, 0.00615302}, {41.25, 0.00614808}, {42., 0.00614276}, {42.75, 0.00613709},
 {43.5, 0.0061311}, {44.25, 0.0061248}, {45., 0.00611823}, {45.75, 0.0061114},
 {46.5, 0.00610432}, {47.25, 0.00609703}, {48., 0.00608952}, {48.75, 0.00608182},
 {49.5, 0.00607394}, {50.25, 0.00606589}, {51., 0.00605767}, {51.75, 0.00604931},
 {52.5, 0.00604081}, {53.25, 0.00603218}, {54., 0.00602342}, {54.75, 0.00601455},
 {55.5, 0.00600556}, {56.25, 0.00599647}, {57., 0.00598728}, {57.75, 0.005978},
 {58.5, 0.00596864}, {59.25, 0.00595918}, {60., 0.00594965}, {60, 0.00594965}}
```

```
In[•]:= curr3 = yValues3 + realcorrection3;
        pair3 = Transpose[{qs3, curr3}];
        s3 =
         ListPlot[pair3, PlotMarkers → {Graphics[{EdgeForm[Black], White, Disk[]}], 7},
          FrameLabel → {{Row[{"Energy, ", Style["ϵ", Italic], " (meV)"}], ""},
            {Row[{"Momentum, ", Style["q", Italic], " (μm^-1)"}], ""}} , Frame → True,
          FrameTicks → {{{{0, "0.0"}, {0.002, "", {0.003, 0}}, {0.004, "4.0"}, {0.006,
                "", {0.003, 0}}, {0.008, "8.0"}, {0.01, "", {0.003, 0}}, {0.012, "12.0"}},
              {{0, "0.0"}, {0.002, "", {0.003, 0}}, {0.004, "4.0"}, {0.006, "", {0.003, 0}},
               {0.008, "8.0"}, {0.01, "", {0.003, 0}}, {0.012, "12.0"}}},
             {{{10, "10"}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
               {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
               {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
              {{10, "10"}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}},
               {30, ""}, {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
               {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
          PlotRange → {{11, 61}, {-0.0003, 0.012}}, PlotLegends → {"CsPbBr1.5Cl1.5"}]
```

Out[•]=




```
In[•]:= qs3 = Range[10.75, 60, 1];

In[•]:= yValues3 = middleSolution /@ qs3;
```

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

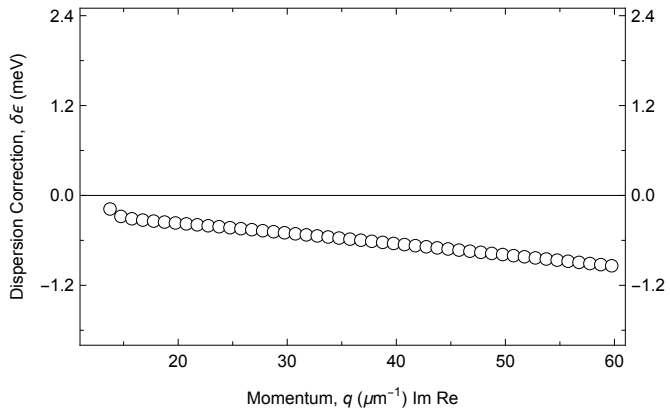
Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

General : Further output of Solve::ratnz will be suppressed during this calculation.

```
In[•]:= xyPairs3 = Transpose[{qs3, yValues3}];
```

```
In[•]:= realcorrection3 = DR @@@ xyPairs3;

In[•]:= imaginarycorrection3 = DI @@@ xyPairs3;

In[•]:= qandreal3 = Transpose[{qs3, realcorrection3}];

In[•]:= qversusreal3 =
         ListPlot[qandreal3, PlotMarkers → {Graphics[{EdgeForm[Black], White, Disk[]}], 7},
          FrameLabel → {{"Dispersion Correction, δϵ (meV)", ""},
            {Row[{"Momentum, ", Style["q", Italic], " (μm^-1) Im Re"}], ""}},
          Frame → True, FrameTicks → {{{{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"},
              {-0.0006, "", {0.003, 0}}, {0, "0.0"}, {0.0006, "", {0.003, 0}},
              {0.0012, "1.2"}, {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}},
             {{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"}, {-0.0006, "", {0.003, 0}},
              {0, "0.0"}, {0.0006, "", {0.003, 0}}, {0.0012, "1.2"},
              {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}}},
            {{{10, ""}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
              {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
              {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
             {{10, ""}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}}, {30, ""},
              {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
              {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
          PlotRange → {{11, 61}, {-0.002, 0.0025}}]
```

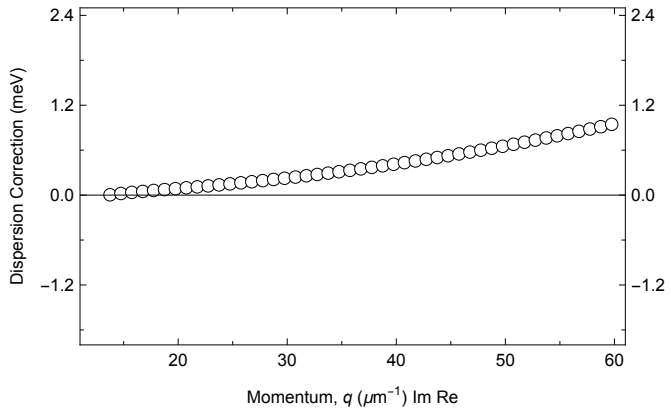
Out[•]=




```
In[•]:= qandimaginary3 = Transpose[{qs3, imaginarycorrection3}];
```

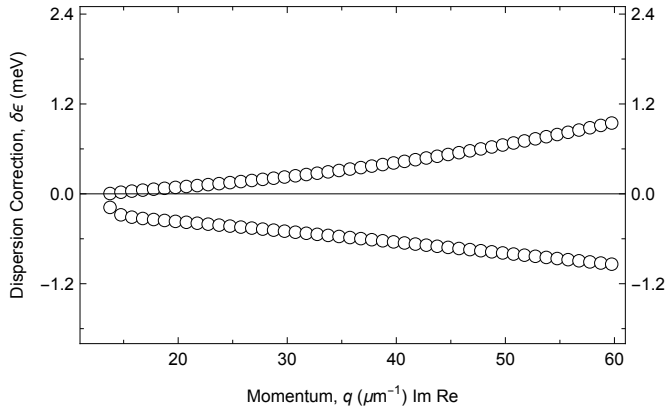
In[ ]:=
```
qversusimaginary3 = ListPlot[qandimaginary3,
  PlotMarkers → {Graphics[{EdgeForm[Black], White, Disk[]}], 7},
  FrameLabel → {{"Dispersion Correction (meV)", ""},
    {Row[{"Momentum, ", Style["q", Italic], " (μm^-1) Im Re"}], ""}},
  Frame → True, FrameTicks → {{{{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"},
      {-0.0006, "", {0.003, 0}}, {0, "0.0"}, {0.0006, "", {0.003, 0}},
      {0.0012, "1.2"}, {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}},
     {{-0.0018, "", {0.003, 0}}, {-0.0012, "-1.2"}, {-0.0006, "", {0.003, 0}},
      {0, "0.0"}, {0.0006, "", {0.003, 0}}, {0.0012, "1.2"},
      {0.0018, "", {0.003, 0}}, {0.0024, "2.4"}}},
    {{{10, ""}, {15, "", {0.003, 0}}, {20, "20"}, {25, "", {0.003, 0}},
      {30, "30"}, {35, "", {0.003, 0}}, {40, "40"}, {45, "", {0.003, 0}}, {50, "50"},
      {55, "", {0.003, 0}}, {60, "60"}, {65, "", {0.003, 0}}, {70, "70"}},
     {{10, ""}, {15, "", {0.003, 0}}, {20, ""}, {25, "", {0.003, 0}}, {30, ""},
      {35, "", {0.003, 0}}, {40, ""}, {45, "", {0.003, 0}}, {50, ""},
      {55, "", {0.003, 0}}, {60, ""}, {65, "", {0.003, 0}}, {70, ""}}}},
  PlotRange → {{11, 61}, {-0.002, 0.0025}}]
```

Out[ ]=



In[ ]:=
```
y3 = Show[qversusreal3, qversusimaginary3]
```

Out[ ]=



In[ ]:=

In[ ]:= frontV3 = Range[0.01, 11, 0.25];

In[ ]:= firstHalfV3 = Range[10.8, 11.8, 0.1];

In[ ]:= middleV3 = Range[11.8, 12.7, 0.015];

In[ ]:=

In[ ]:= thirdV3 = Range[12.7, 14, 0.09];

In[ ]:= secondHalfV3 = Range[14, 27, 0.15];

In[ ]:= qsV3 = Join[frontV3, firstHalfV3, middleV3, thirdV3, secondHalfV3];

In[ ]:= yValuesforV3 = middleSolution /@ qsV3;

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

Solve : Solve was unable to solve the system with inexact coefficients. The answer was obtained by solving a corresponding exact system and numericizing the result.

General : Further output of Solve::ratnz will be suppressed during this calculation.

In[ ]:= xyPairsForV3 = Transpose[{qsV3, yValuesforV3}];

In[ ]:= Velocities3 = V @@@ xyPairsForV3;

In[ ]:= VasFuncQ3 = Transpose[{qsV3, Re[Velocities3] / (c * h)}]

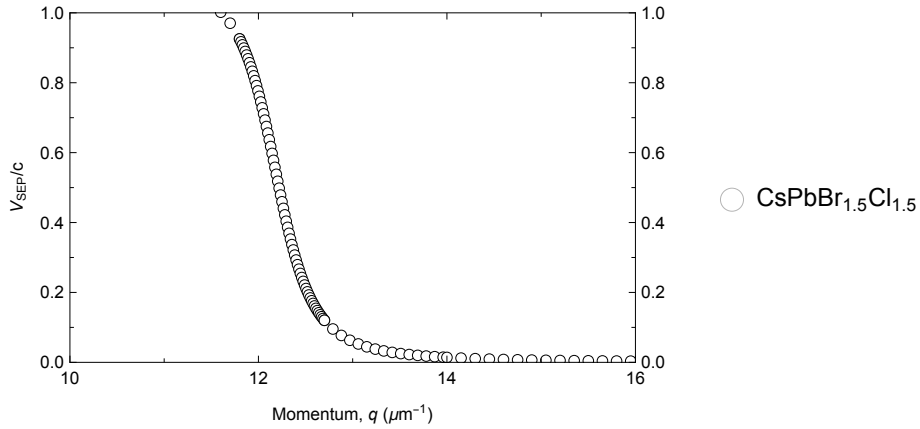
Out[ ]=

{{0.01, 1.10489}, {0.26, 1.10487}, {0.51, 1.10486}, {0.76, 1.10484}, {1.01, 1.10483},
 {1.26, 1.10481}, {1.51, 1.10479}, {1.76, 1.10477}, {2.01, 1.10475},
 {2.26, 1.10472}, {2.51, 1.1047}, {2.76, 1.10467}, {3.01, 1.10464}, {3.26, 1.10461},
 {3.51, 1.10458}, {3.76, 1.10454}, {4.01, 1.1045}, {4.26, 1.10445}, {4.51, 1.1044},
 {4.76, 1.10435}, {5.01, 1.10428}, {5.26, 1.10422}, {5.51, 1.10414},
 {5.76, 1.10406}, {6.01, 1.10396}, {6.26, 1.10386}, {6.51, 1.10373},
 {6.76, 1.1036}, {7.01, 1.10344}, {7.26, 1.10325}, {7.51, 1.10304},
 {7.76, 1.10279}, {8.01, 1.10249}, {8.26, 1.10214}, {8.51, 1.10171},
 {8.76, 1.10118}, {9.01, 1.10053}, {9.26, 1.09971}, {9.51, 1.09865},
 {9.76, 1.09726}, {10.01, 1.09537}, {10.26, 1.09273}, {10.51, 1.08889},
 {10.76, 1.083}, {10.8, 1.08178}, {10.9, 1.07825}, {11., 1.07388}, {11.1, 1.06839},
 {11.2, 1.06141}, {11.3, 1.05234}, {11.4, 1.04035}, {11.5, 1.02415}, {11.6, 1.0018},
 {11.7, 0.970315}, {11.8, 0.92532}, {11.8, 0.92532}, {11.815, 0.917058},
 {11.83, 0.908341}, {11.845, 0.899144}, {11.86, 0.889448}, {11.875, 0.87923},
 {11.89, 0.86847}, {11.905, 0.857148}, {11.92, 0.845248}, {11.935, 0.832753},
 {11.95, 0.819652}, {11.965, 0.805937}, {11.98, 0.791602}, {11.995, 0.776647},
 {12.01, 0.76108}, {12.025, 0.744912}, {12.04, 0.728162}, {12.055, 0.710856},

{12.07, 0.693027}, {12.085, 0.674717}, {12.1, 0.655974}, {12.115, 0.636854},
{12.13, 0.617419}, {12.145, 0.597738}, {12.16, 0.577881}, {12.175, 0.557926},
{12.19, 0.53795}, {12.205, 0.518031}, {12.22, 0.498247}, {12.235, 0.47867},
{12.25, 0.459373}, {12.265, 0.440421}, {12.28, 0.421872}, {12.295, 0.40378},
{12.31, 0.386188}, {12.325, 0.369136}, {12.34, 0.352653}, {12.355, 0.336761},
{12.37, 0.321477}, {12.385, 0.306809}, {12.4, 0.292761}, {12.415, 0.279332},
{12.43, 0.266513}, {12.445, 0.254296}, {12.46, 0.242665}, {12.475, 0.231606},
{12.49, 0.2211}, {12.505, 0.211126}, {12.52, 0.201664}, {12.535, 0.192692},
{12.55, 0.184189}, {12.565, 0.176132}, {12.58, 0.168498}, {12.595, 0.161268},
{12.61, 0.154419}, {12.625, 0.147932}, {12.64, 0.141786}, {12.655, 0.135962},
{12.67, 0.130444}, {12.685, 0.125212}, {12.7, 0.120252}, {12.7, 0.120252},
{12.79, 0.0953648}, {12.88, 0.0769773}, {12.97, 0.0631587}, {13.06, 0.0525905},
{13.15, 0.0443706}, {13.24, 0.0378759}, {13.33, 0.0326696}, {13.42, 0.0284408},
{13.51, 0.0250443}, {13.6, 0.0222867}, {13.69, 0.0199213}, {13.78, 0.017898},
{13.87, 0.0161596}, {13.96, 0.0146571}, {14., 0.0140544}, {14.15, 0.0120911},
{14.3, 0.0105065}, {14.45, 0.00921009}, {14.6, 0.00813649}, {14.75, 0.00723774},
{14.9, 0.00647801}, {15.05, 0.00583016}, {15.2, 0.00527332}, {15.35, 0.00479126},
{15.5, 0.0043712}, {15.65, 0.00400297}, {15.8, 0.00367839}, {15.95, 0.00339083},
{16.1, 0.00313489}, {16.25, 0.00290609}, {16.4, 0.00270074}, {16.55, 0.00251573},
{16.7, 0.00234848}, {16.85, 0.00219678}, {17., 0.00205876}, {17.15, 0.00193283},
{17.3, 0.00181762}, {17.45, 0.00171194}, {17.6, 0.00161478}, {17.75, 0.00152524},
{17.9, 0.00144254}, {18.05, 0.00136602}, {18.2, 0.00129506}, {18.35, 0.00122915},
{18.5, 0.00116781}, {18.65, 0.00111064}, {18.8, 0.00105726}, {18.95, 0.00100735},
{19.1, 0.000960608}, {19.25, 0.000916781}, {19.4, 0.000875628},
{19.55, 0.000836937}, {19.7, 0.000800515}, {19.85, 0.00076619}, {20., 0.000733803},
{20.15, 0.000703211}, {20.3, 0.000674286}, {20.45, 0.000646908},
{20.6, 0.000620969}, {20.75, 0.00059637}, {20.9, 0.000573022}, {21.05, 0.00055084},
{21.2, 0.000529749}, {21.35, 0.000509679}, {21.5, 0.000490566},
{21.65, 0.000472348}, {21.8, 0.000454973}, {21.95, 0.000438388},
{22.1, 0.000422548}, {22.25, 0.000407407}, {22.4, 0.000392926},
{22.55, 0.000379068}, {22.7, 0.000365797}, {22.85, 0.00035308},
{23., 0.000340888}, {23.15, 0.000329192}, {23.3, 0.000317966},
{23.45, 0.000307185}, {23.6, 0.000296826}, {23.75, 0.000286868},
{23.9, 0.00027729}, {24.05, 0.000268073}, {24.2, 0.000259199},
{24.35, 0.000250653}, {24.5, 0.000242417}, {24.65, 0.000234478},
{24.8, 0.00022682}, {24.95, 0.000219433}, {25.1, 0.000212301},
{25.25, 0.000205416}, {25.4, 0.000198764}, {25.55, 0.000192336},
{25.7, 0.000186122}, {25.85, 0.000180112}, {26., 0.000174299},
{26.15, 0.000168673}, {26.3, 0.000163227}, {26.45, 0.000157952},
{26.6, 0.000152843}, {26.75, 0.000147892}, {26.9, 0.000143093}}

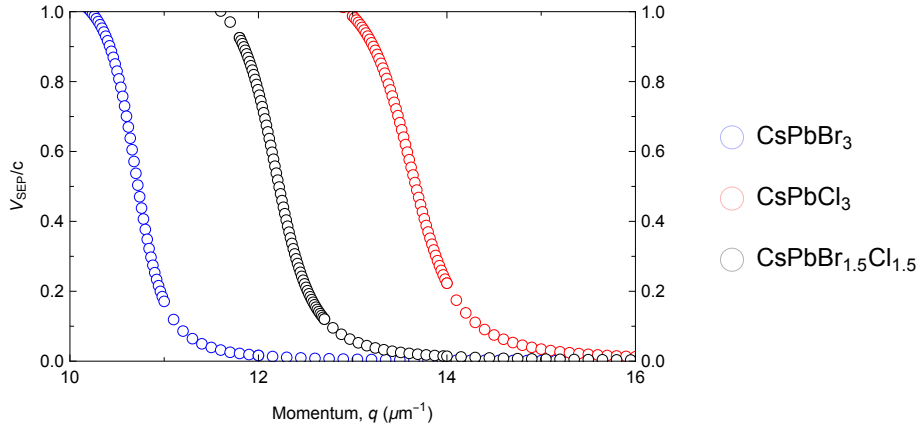
In[ ]:=
```
v3 = ListPlot[VasFuncQ3,
  PlotMarkers → {Graphics[{EdgeForm[Black], White, Disk[]}], 6}, FrameLabel →
   {{"V_SEP/c", ""}, {Row[{"Momentum, ", Style["q", Italic], " (μm^-1)"}], ""}},
  Frame → True, FrameTicks → {{{{0.0, "0.0"}, {0.1, "", {0.003, 0}}, {0.2, "0.2"},
      {0.3, "", {0.003, 0}}, {0.4, "0.4"}, {0.5, "", {0.003, 0}}, {0.6, "0.6"},
      {0.7, "", {0.003, 0}}, {0.8, "0.8"}, {0.9, "", {0.003, 0}}, {1.0, "1.0"}},
     {{0.0, "0.0"}, {0.1, "", {0.003, 0}}, {0.2, "0.2"}, {0.3, "", {0.003, 0}},
      {0.4, "0.4"}, {0.5, "", {0.003, 0}}, {0.6, "0.6"}, {0.7, "", {0.003, 0}},
      {0.8, "0.8"}, {0.9, "", {0.003, 0}}, {1.0, "1.0"}}},
    {{{8, "8"}, {9, "", {0.003, 0}}, {10, "10"}, {11, "", {0.003, 0}},
      {12, "12"}, {13, "", {0.003, 0}}, {14, "14"}, {15, "", {0.003, 0}},
      {16, "16"}, {17, "", {0.003, 0}}, {18, "18"}}, {{8, ""}, {9, "", {0.003, 0}},
      {10, ""}, {11, "", {0.003, 0}}, {12, ""}, {13, "", {0.003, 0}}, {14, ""},
      {15, "", {0.003, 0}}, {16, ""}, {17, "", {0.003, 0}}, {18, ""}}}},
  PlotLegends → {"CsPbBr1.5Cl1.5"}, PlotRange → {{10, 16}, {0, 1}}]
```

Out[ ]=



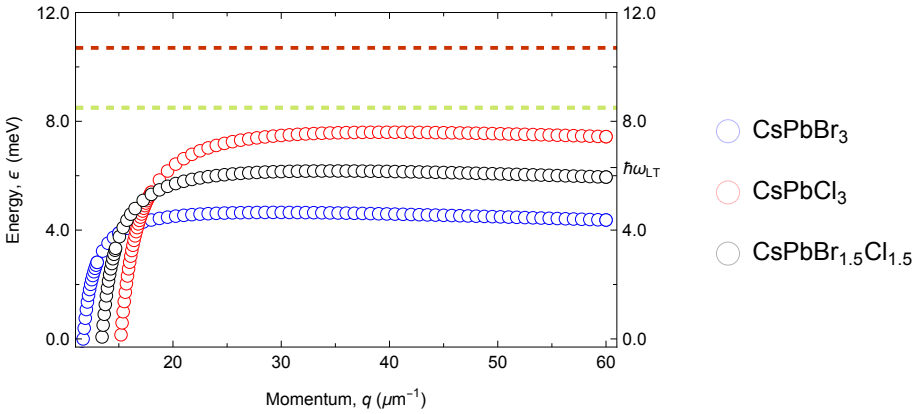
In[ ]:=
```
FinalVelocities = Show[v1, v2, v3]
```

Out[ ]=



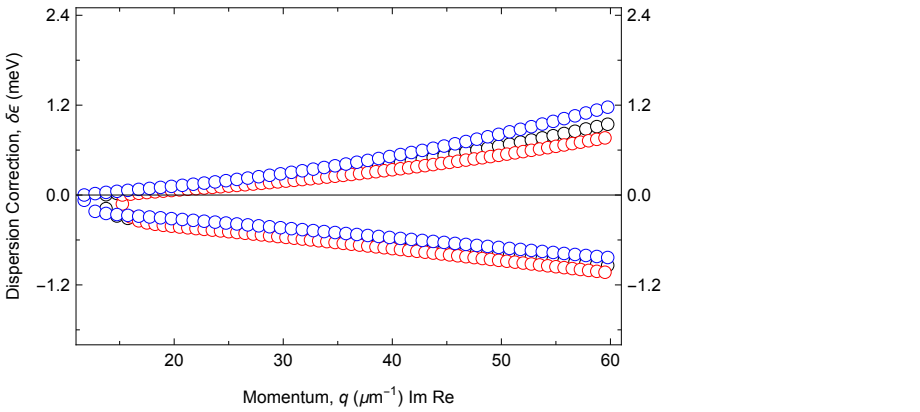
```
In[ ]:= BrLT = ContourPlot[y == 0.0063, {x, 11, 61},
          {y, -0.0003, 0.011}, PlotRange → {{11, 61}, {-0.0003, 0.012}},
          ContourStyle → {Dashed, ColorData["DeepSeaColors"][0.2]}]

In[ ]:= ClLT = ContourPlot[y == 0.0107, {x, 11, 61},
          {y, -0.0003, 0.011}, PlotRange → {{11, 61}, {-0.0003, 0.012}},
          ContourStyle → {Dashed, ColorData[80, 1]}]

In[ ]:= BothLT = BrLT = ContourPlot[y == (0.0063 + 0.0107) / 2, {x, 11, 61},
           {y, -0.0003, 0.011}, PlotRange → {{11, 61}, {-0.0003, 0.012}},
           ContourStyle → {Dashed, ColorData[45, 45]}]

In[ ]:= FinalDispersions = Show[s1, s2, s3, ClLT, BothLT, BrLT]
```

Out[ ]=




```
In[ ]:= FinalCorrections = Show[qversusreal3, qversusimaginary3,
          qversusreal2, qversusimaginary2, qversusreal1, qversusimaginary1]
```

Out[ ]=




```
In[ ]:=
```