```
matrix as in notes by Geshjkenbein, p.6 ff *)
  In[31]:= Clear[ell, q, p, epsilon, m]
  m(32):= ell := {{1, 1}, {Iq, -Iq}} (* matrix L *)
  In[33]:= MatrixForm[ell]
Out[33]//MatrixForm=
         \begin{pmatrix} 1 & 1 \\ i & q & -i & q \end{pmatrix}
  ln[34]:= V := \{\{1, 0\}, \{epsilon, 1\}\}  (* matrix V,
           epsilon as defined in Section 2.2 *)
  In[35]:= MatrixForm[v]
Out[35]//MatrixForm=
          \begin{pmatrix} 1 & 0 \\ epsilon & 1 \end{pmatrix}
  ln[36] = p := \{ \{ Exp[Iq], 0 \}, \{ 0, Exp[-Iq] \} \}
            (* matrix P, called T in Geshjkenbein *)
  In[37]:= MatrixForm[p]
Out[37]//MatrixForm=

\left(\begin{array}{ccc}
\mathbb{C}^{\dot{1}} & \mathbf{q} & \mathbf{0} \\
\mathbf{0} & \mathbb{C}^{-\dot{1}} & \mathbf{q}
\end{array}\right)

  | t := p.Inverse[ell, Method -> "CofactorExpansion"].
             v.ell (* transfer matrix T *)
  In[39]:= MatrixForm[t]
Out[39]//MatrixForm=
           \begin{array}{cccc} \mathbb{e}^{\frac{i}{q}} \, q & & \frac{i \, e^{i \, q} \, epsilon}{2 \, q} & & -\frac{i \, e^{i \, q} \, epsilon}{2 \, q} \\ & & \frac{i \, e^{-i \, q} \, epsilon}{2 \, q} & & \mathbb{e}^{-i \, q} \, + \frac{i \, e^{-i \, q} \, epsilon}{2 \, q} \end{array} \right)
  In[28]:= Det[t]
  Out[28]= 1
         (* Eigenvectors of transfer matrix t *)
```

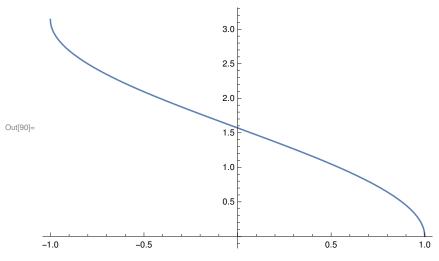
(* Kronig-Penney model using transfer

```
In[42]:= Eigenvectors[t]
\text{Out}[42] = \left\{ \left\{ -\left( \left( \text{epsilon} + \text{e}^{2 \text{ i } \text{q}} \text{ epsilon} - 2 \text{ i } \text{q} + 2 \text{ i } \text{e}^{2 \text{ i } \text{q}} \text{ q} - \right) \right\} \right\} \right\}
                    i\sqrt{\left(-16\,\mathrm{e}^{2\,i\,q}\,\mathsf{q}^2+\left(-\,i\,\,\mathsf{epsilon}+i\,\,\mathrm{e}^{2\,i\,q}\,\,\mathsf{epsilon}-2\right)}
                                  q - 2 e^{2 i q} q)^{2} / (2 epsilon), 1,
        \left\{-\left(\left(\text{epsilon} + e^{2 i q} \text{epsilon} - 2 i q + 2 i e^{2 i q} q + \right)\right\}\right\}
                   \dot{\mathbb{1}} \sqrt{\left(-16 e^{2 \dot{\mathbb{1}} q} q^2 + \left(-\dot{\mathbb{1}} epsilon + \dot{\mathbb{1}} e^{2 \dot{\mathbb{1}} q} epsilon - 2\right)}
                                  q - 2 e^{2 i q} q)^2) / (2 epsilon), 1}
       (* pasted from above *)
In[43]:= va1[q , epsilon ] :=
        \left\{-\left(\left(\text{epsilon} + e^{2iq} \text{epsilon} - 2iq + 2ie^{2iq}q - \right)\right\}\right\}
                   i \sqrt{\left(-16 e^{2 i q} q^2 + \left(-i epsilon + i e^{2 i q} epsilon - 2\right)\right)}
                                  q - 2e^{2iq}q)^2))/(2epsilon)), 1
In[44]:= v1[q , epsilon ] :=
        va1[q, epsilon] / Norm[va1[q, epsilon]] (* normalized *)
In[45]:= va2[q_, epsilon_] :=
        \{-((epsilon + e^{2iq} epsilon - 2iq + 2ie^{2iq}q +
                   i \sqrt{(-16 e^{2 i q} q^2 + (-i epsilon + i e^{2 i q} epsilon − 2)}
                                  q - 2 e^{2 i q} q)^{2}) / (2 epsilon), 1
v2[q_, epsilon_] := va2[q, epsilon] / Norm[va2[q, epsilon]]
       (* Simplified form of above eigenvectors *)
 ln[64] = qq[q, epsilon] := Cos[q] + (epsilon/(2q)) Sin[q]
ww[q , epsilon ] := -Cos[q] + (2 q / epsilon) Sin[q]
In[66]:= vv1[q , epsilon ] := {Exp[Iq] (ww[q, epsilon] +
                (2 q / epsilon) Sqrt[1 - qq[q, epsilon] ^ 2]), 1}
```

```
\[ vv2[q , epsilon ] := {Exp[I q] (ww[q, epsilon] -
           (2 q / epsilon) Sqrt[1 - qq[q, epsilon] ^ 2]), 1}
In[56]:= (* Check that vv1 = va1, vv2 = va2 *)
ln[68]:= va1[0.7, 0.1]
Out[68]= \{12.5798 + 10.5958 \, i, 1\}
ln[69]:= VV1[0.7, 0.1]
Out[69]= \{12.5798 + 10.5958 \, \dot{\mathbb{1}}, 1\}
ln[70] = va2[0.7, 0.1]
Out[70]= \{0.0465017 + 0.0391679 i, 1\}
ln[71] = vv2[0.7, 0.1]
Out[71]= \{0.0465017 + 0.0391679 i, 1\}
    (* End check *)
In[74]:= (* Modified,
    normalized eigenvectors to be used in the following *)
In[75]:= v1norm[q , epsilon ] :=
     vv1[q, epsilon] / Norm[vv1[q, epsilon]]
w2norm[q , epsilon ] := Exp[-Iq] vv2[q, epsilon] /
        Norm[vv2[q, epsilon]] (* note factor Exp[-I q] *)
ln[77]:= (* v1norm[[1]]+v1norm[[2]] and v2norm[[1]]+
     v2norm[[2]] are complex conjugate,
       but only with factor Exp[-I q] in v2norm
     included. This is the modification. *)
In[79]:= v1norm[0.7, 0.1][[1]] + v1norm[0.7, 0.1][[2]]
Out[79]= 0.82412 + 0.64303 i
```

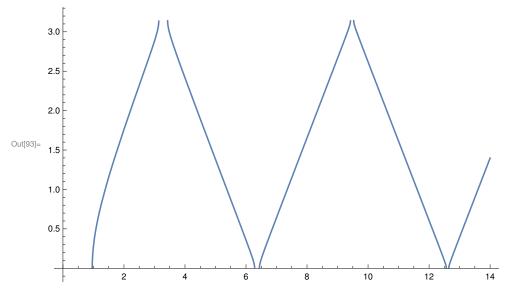
```
v2norm[0.7, 0.1][[1]] + v2norm[0.7, 0.1][[2]]
 Out[80]= 0.82412 - 0.64303 i
  (* alternative form of v2norm, further simplified *)
  ww[q, epsilon] := {ww[q, epsilon] -
                                        (2 q / epsilon) Sqrt[1 - qq[q, epsilon] ^2], Exp[-Iq]}
  In[83]:= v2normalt[q_, epsilon_] :=
                           vv2alt[q, epsilon] / Norm[vv2alt[q, epsilon]]
  In[84]:= v2normalt[0.7, 0.1][[1]] + v2normalt[0.7, 0.1][[2]]
 Out[84]= 0.82412 - 0.64303 i
                      (* Eigenvalues mu of transfer matrix t,
                     cp. Geshkenbein, Eq. (50) *)
  In[88]:= Eigenvalues[t]
Out[88]= \left\{ \frac{1}{4 \, \mathsf{a}} \right\}
                          \left(-i \text{ epsilon} + i e^{2iq} \text{ epsilon} - 2q - 2e^{2iq}q\right)^2\right), \frac{1}{4q}
                         \text{e}^{-\text{i}\;q}\;\left(\text{i}\;\text{epsilon}\;-\;\text{i}\;\text{e}^{2\;\text{i}\;q}\;\text{epsilon}\;+\;2\;q\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q\;+\;\sqrt{\;\left(-\,16\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q\;+\;\sqrt{\;\left(-\,16\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q\;+\;\sqrt{\;\left(-\,16\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^{2\;\text{i}\;q}\;q^2\;+\;2\;\text{e}^
                                                                \left(-i \text{ epsilon} + i e^{2iq} \text{ epsilon} - 2q - 2e^{2iq}q\right)^2\right)
                      (* => mu = exp(+/- i k),
                     cos(k) = cos(q) + epsilon/(2q) sin(q) =: Q(q) *)
```





```
(* Illustration: plot band structure q(k) =
omega(k)/v for -Pi<k<Pi in reduced zone scheme *)</pre>
(* for epsilon = 1 *)
```

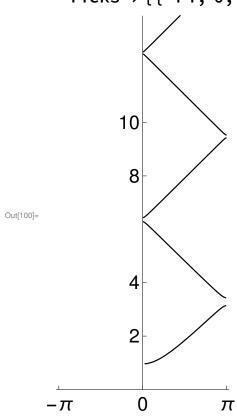
```
[n[93]:= Plot[kk[q, 1], {q, 0, 14}] (* function k(q),
   range 0 < k < Pi, epsilon = 1 *)</pre>
```



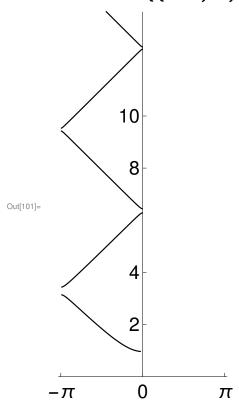
In[94]:= kq[q_, epsilon_] := If[Abs[qq[q, epsilon]] < 1, kk[q, epsilon], 100]</pre> (* k(q), allow only |q|<1 *)

(* use parametric plot to plot inverse function q(k) *)

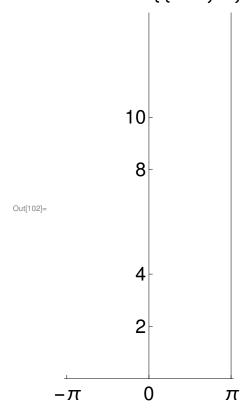
In[100]:= pos = ParametricPlot[{kq[q, 1], q}, {q, 0, 14}, PlotRange $\rightarrow \{\{-Pi - 0.1, Pi + 0.1\}, \{0, 14\}\},\$ PlotStyle → {{Black, Thickness[0.007]}}, AxesStyle → Directive[20], Ticks $\rightarrow \{\{-Pi, 0, Pi\}, \{2, 4, 8, 10\}\}\}$



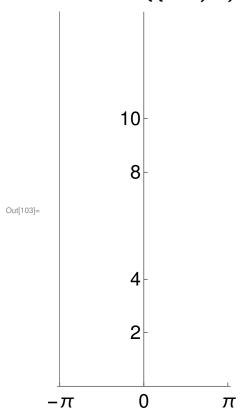
 $lo[101] = neg = ParametricPlot[{-kq[q, 1], q}, {q, 0, 14},$ PlotRange $\rightarrow \{\{-Pi - 0.1, Pi + 0.1\}, \{0, 14\}\},\$ PlotStyle → {{Black, Thickness[0.007]}}, AxesStyle → Directive[20], Ticks \rightarrow {{-Pi, 0, Pi}, {2, 4, 8, 10}}]



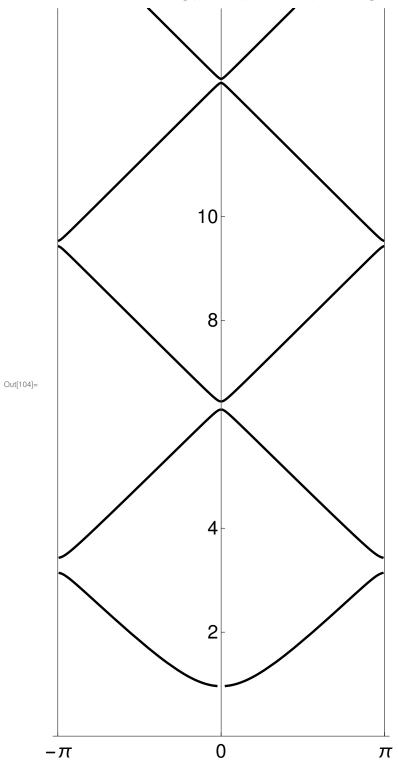
```
In[102]:= pipos = ParametricPlot[{Pi, q}, {q, 0, 14},
       PlotRange \rightarrow \{\{-Pi - 0.1, Pi + 0.1\}, \{0, 14\}\},\
       PlotStyle → {{Black, Thickness[0.0015]}},
       AxesStyle → Directive[20],
       Ticks \rightarrow {{-Pi, 0, Pi}, {2, 4, 8, 10}}]
```



In[103]:= pineg = ParametricPlot[{-Pi, q}, {q, 0, 14}, PlotRange $\rightarrow \{\{-Pi - 0.1, Pi + 0.1\}, \{0, 14\}\},\$ PlotStyle → {{Black, Thickness[0.0015]}}, AxesStyle → Directive[20], Ticks \rightarrow {{-Pi, 0, Pi}, {2, 4, 8, 10}}]



In[104]:= band = Show[neg, pos, pipos, pineg]



```
In[105]= Export["bs.png", band, ImageResolution → 300]
Out[105]= bs.png
    (* End Illustration *)
    (* Bloch functions Phi(x)
     with additional normalization *)
    (* allow only |q|<1 *)
    (* in what follows: index 1 = +k, index 2 = -k *)
log_{i=1} = exp1[q, epsilon, n] := If[Abs[qq[q, epsilon]] < 1,
      Exp[Ikk[q, epsilon]n], 0] (* k1 > 0 *)
In[107]:= exp2[q_, epsilon_, n_] := If[Abs[qq[q, epsilon]] < 1,</pre>
      Exp[-Ikk[q, epsilon] n], 0] (* k2 = -k1 < 0 *)
    (* phi1raw, phi2raw not correctly normalized,
    missing normalization factors norm1, norm2 below *)
| In[108]:= phi1raw[x_, n_, q_, epsilon_] :=
     exp1[q, epsilon, n] (v1norm[q, epsilon][[1]] Exp[I q (x - n)] +
          v1norm[q, epsilon][[2]] Exp[-Iq(x-n)]) /
        (v1norm[q, epsilon][[1]] + v1norm[q, epsilon][[2]])
n[109]:= phi2raw[x_, n_, q_, epsilon_] :=
     exp2[q, epsilon, n] (v2norm[q, epsilon][[1]] Exp[I q (x - n)] +
          v2norm[q, epsilon][[2]] Exp[-Iq(x-n)]) /
        (v2norm[q, epsilon][[1]] + v2norm[q, epsilon][[2]])
```

(* functions u(x) for 0<x<1, then periodically extended *)

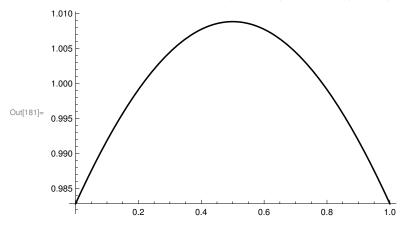
```
in[110]:= u1raw[x_, q_, epsilon_] :=
      (v1norm[q, epsilon][[1]] Exp[I (q - kk[q, epsilon]) (x - 1)] +
         v1norm[q, epsilon][[2]]
          Exp[-I (q + kk[q, epsilon]) (x - 1)]) /
       (v1norm[q, epsilon][[1]] + v1norm[q, epsilon][[2]])
m[iii]= norm1[q , epsilon ] := Sqrt[NIntegrate[u1raw[x, q, epsilon]
         Conjugate [u1raw[x, q, epsilon]], \{x, 0, 1\}]
In[112]:= u1[x_, q_, epsilon_] :=
     u1raw[x, q, epsilon] / norm1[q, epsilon]
In[113]= NIntegrate[u1[x, 0.3, 0.7] Conjugate[u1[x, 0.3, 0.7]],
     {x, 0, 1}] (* u1 correctly normalized *)
Out[113]= 1.
In[114]:= u2raw[x , q , epsilon ] :=
      (v2norm[q, epsilon][[1]] Exp[I (q+kk[q, epsilon]) (x-1)] +
         v2norm[q, epsilon][[2]]
          Exp[-I (q - kk[q, epsilon]) (x - 1)]) /
       (v2norm[q, epsilon][[1]] + v2norm[q, epsilon][[2]])
տ[115]≔ norm2[q_, epsilon_] := Sqrt[NIntegrate[u2raw[x, q, epsilon]
         Conjugate[u2raw[x, q, epsilon]], {x, 0, 1}]]
ln[116]:= u2[x, q, epsilon] :=
     u2raw[x, q, epsilon] / norm2[q, epsilon]
m[117] = NIntegrate[u2[x, 0.3, 0.7] Conjugate[u2[x, 0.3, 0.7]],
     {x, 0, 1}] (* u2 correctly normalized *)
Out[117]= 1.
    (* functions c(q), d(q) *)
h[121]:= u1prime[x_, q_, epsilon_] :=
     Derivative[1, 0, 0][u1raw][x, q, epsilon] / norm1[q, epsilon]
```

```
h[119]:= u2prime[x_, q_, epsilon_] :=
                          Derivative[1, 0, 0] [u2raw] [x, q, epsilon] / norm2[q, epsilon]
                    c[q , epsilon ] := u1[0, q, epsilon] (* cal C in thesis *)
                      (* c real and equal for (1), (2) *)
 ln[122] = c[0.9, 0.2]
Out[122]= 0.982811 - 5.4557 \times 10^{-17} \ \text{i}
 ln[123] = u2[0, 0.9, 0.2]
Out[123]= 0.982811 - 1.85494 \times 10^{-15} i
 ln[124] = c[2, 3]
Out[124]= 0.762883 + 3.46945 \times 10^{-17} i
 ln[125] = u2[0, 2, 3]
Out[125]= 0.762883 - 4.16334 \times 10^{-17} i
 In[126]:= d[q_, epsilon_] :=
                          u1prime[0, q, epsilon] (* cal D in thesis *)
                      (* d complex and conjugate for (1), (2) *)
 ln[127] = d[0.9, 0.2]
Out[127]= 0.0982811 + 0.0269644 i
 In[128]:= u2prime[0, 0.9, 0.2]
Out[128]= 0.0982811 - 0.0269644 i
 ln[129]:= d[2, 3]
Out[129]= 1.14432 + 0.624518 \pm 0.62418 \pm 0.02418 \pm 0.
 In[130]:= u2prime[0, 2, 3]
Out[130]= 1.14432 - 0.624518 i
```

```
(* Note: For our calculation we
       need C and D as functions of k instead *)
     (* of q=omega. For this we need the
       function q(k) which is the inverse
    (* of the function k(q). See illustration
     at the beginning of the notebook. *)
    (* If we have q(k) then c[k, epsilon] =
     u1[0, q(k), epsilon] and *)
    (* d[k, epsilon] = uprime1[0, q(k), epsilon] *)
    (* Illustrations and side calculations *)
    (* Properties of u1, u2 and derivatives *)
     (* Show u1(0)=u1(1)=u2(0)=u2(1) and real *)
log(161) = Abs[qq[0.7, 0.3]] (* needs to be <1 *)
Out[161]= 0.902889
ln[162]:= u1[0, 0.7, 0.3] // N
Out[162]= 0.975105 - 1.62388 \times 10^{-16} i
ln[163]:= u1[1, 0.7, 0.3] // N
Out[163]= 0.975105 + 0.1
ln[170] = u2[0, 0.7, 0.3] // N
Out[170]= 0.975105 - 2.16517 \times 10^{-16} i
ln[171] = u2[1, 0.7, 0.3] // N
Out[171]= 0.975105 + 5.41292 \times 10^{-17} i
log(172) = Abs[qq[0.9, 0.2]] (* needs to be <1 *)
Out[172]= 0.708646
```

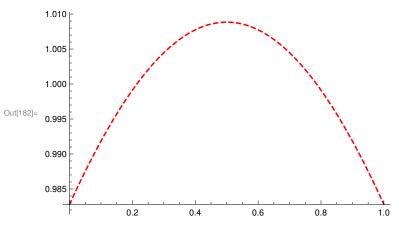
```
ln[173]:= u1[0, 0.9, 0.2] // N
Out[173]= 0.982811 - 5.4557 \times 10^{-17} i
ln[174]:= u1[1, 0.9, 0.2] // N
Out[174]= 0.982811 + 0.1
ln[175] = u2[0, 0.9, 0.2] // N
Out[175]= 0.982811 - 1.85494 \times 10^{-15} i
ln[176] = u2[1, 0.9, 0.2] // N
Out[176]= 0.982811 + 0.1
log(177) = Abs[qq[0.3, 0]] (* needs to be <1 *)
Out[177]= 0.955336
In[142]:= (* Show u1=u2=1 for epsilon=0 *)
ln[143] = u1[0.9, 0.3, 0.0000000001]
Out[143]= 1. - 3.62765 \times 10^{-13} i
ln[144]:= u2[0.9, 0.3, 0.0000000001]
Out[144]= 1. + 4.1371 \times 10<sup>-8</sup> i
log(145)= (* Show: u2 = Conjugate[u1] if Abs[qq]<1 *)
log_{178} = Abs[qq[0.9, 0.2]] (* needs to be <1 *)
Out[178]= 0.708646
ln[179] = u1[0.3, 0.9, 0.2]
Out[179]= 1.00448 + 0.00233511 i
ln[180] = u2[0.3, 0.9, 0.2]
Out[180]= 1.00448 - 0.00233511 i
log(151)= (* plot real part of u(x) for epsilon = 0.2 *)
```

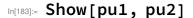
 $ln[181]= pu1 = Plot[Re[u1[x, 0.9, 0.2]], \{x, 0, 1\}, PlotStyle \rightarrow Black]$

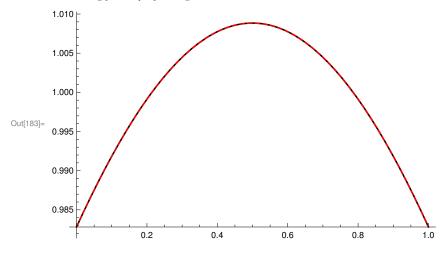


ln[182] = pu2 = Plot[Re[u2[x, 0.9, 0.2]],

 $\{x, 0, 1\}, PlotStyle \rightarrow \{Red, Dashed\}]$

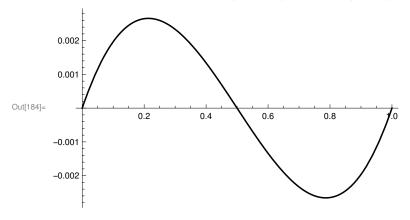




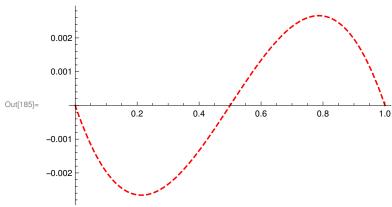


(* plot imaginary part of u(x) *)

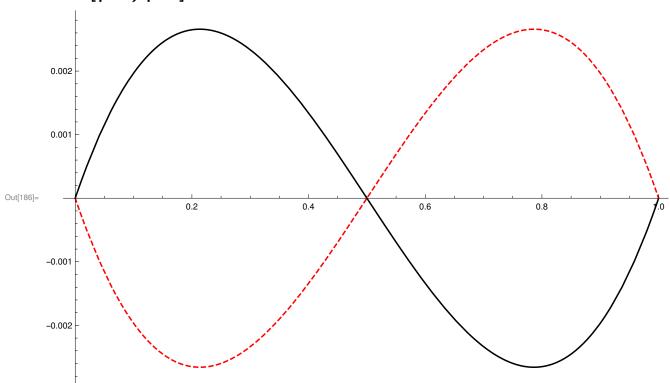
 $ln[184]:= pu3 = Plot[Im[u1[x, 0.9, 0.2]], \{x, 0, 1\}, PlotStyle \rightarrow Black]$



ln[185] = pu4 = Plot[Im[u2[x, 0.9, 0.2]], $\{x, 0, 1\}, PlotStyle \rightarrow \{Red, Dashed\}]$

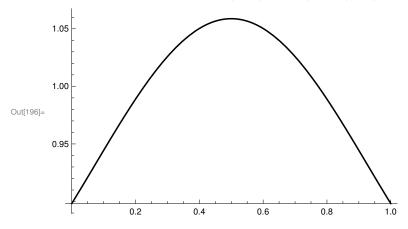






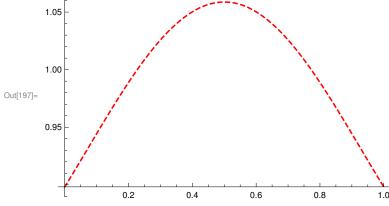
```
(* Illustration: plot u(x) for epsilon = 1 and q=2 *)
In[193]:= Abs[qq[2, 1]] // N (* needs to be <1 *)
Out[193]= 0.188822
In[194]:= u1[0.4, 2, 1]
Out[194]= 1.05025 + 0.0207882 i
In[195]:= u2[0.4, 2, 1]
Out[195]= 1.05025 - 0.0207882 i
     (* plot real part of u(x) *)
```

 $ln[196]:= pu5 = Plot[Re[u1[x, 2, 1]], \{x, 0, 1\}, PlotStyle \rightarrow Black]$

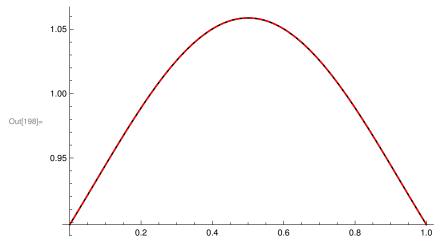


ln[197] = pu6 = Plot[Re[u2[x, 2, 1]],



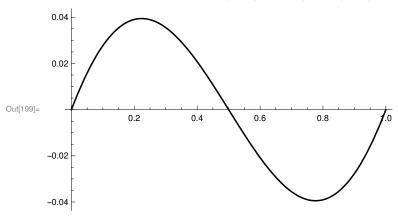


In[198]:= Show[pu5, pu6]

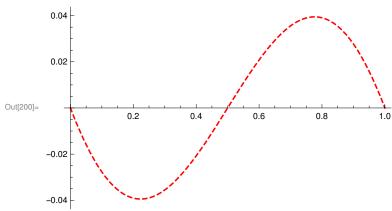


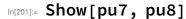
(* plot imaginary part of u(x) *)

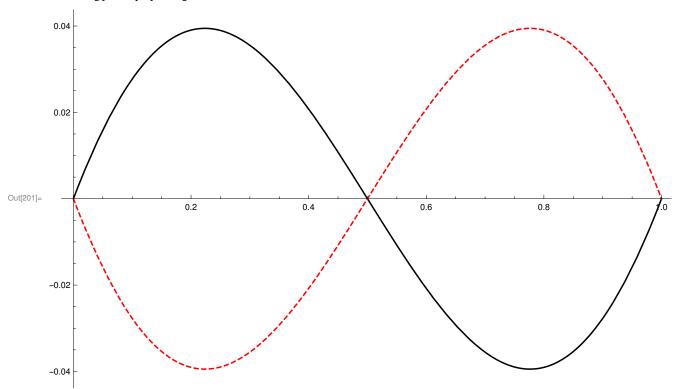
$\label{eq:pu7} \textit{pu7} = \mathsf{Plot}[\mathsf{Im}[\mathsf{u1}[\mathsf{x},\,2,\,1]],\,\{\mathsf{x},\,0,\,1\}\,,\,\mathsf{PlotStyle} \to \mathsf{Black}]$



In[200]:= pu8 = Plot[Im[u2[x, 2, 1]], $\{x, 0, 1\}, PlotStyle \rightarrow \{Red, Dashed\}]$

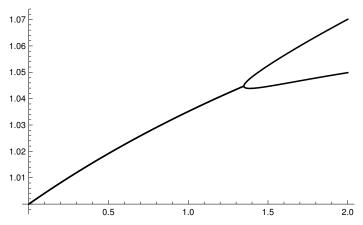




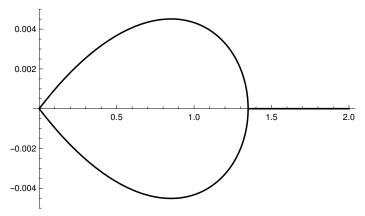


Abs[qq[1.1, 1.348]] (* epsilon=1.348 is critical value for q=1.1 *) 0.999663

Plot[{Re[u1[0.4, 1.1, eps]], Re[u2[0.4, 1.1, eps]]}, {eps, 0, 2}, PlotStyle \rightarrow Black]



Plot[{Im[u1[0.4, 1.1, eps]], Im[u2[0.4, 1.1, eps]]}, {eps, 0, 2}, PlotStyle → Black]



```
(* Show: u2'[0] = Conjugate[u1'[0]] if Abs[qq]<1 *)
Abs[qq[0.9, 0.2]] (* needs to be <1 *)
0.708646
u1prime[0, 0.9, 0.2]
0.0982811 + 0.0269644 i
u2prime[0, 0.9, 0.2]
0.0982811 - 0.0269644 i
Abs[qq[2, 3]] // N (* needs to be <1 *)
0.265826
u1prime[0, 2, 3]
1.14432 + 0.624518 i
```

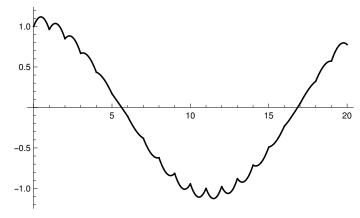
1.14432 - 0.624518 i

u2prime[0, 2, 3]

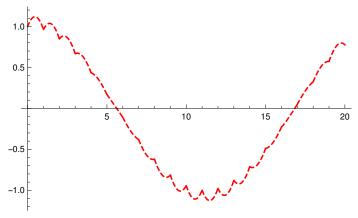
(* END properties of u1, u2 and derivatives *)

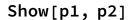
(* Plot real and imaginary parts of Bloch functions Phi_raw(x) *) (* Show Phi 2 raw = complex conjugate Phi 1 raw *) Abs[qq[1, 1]] // N (* needs to be <1 *) 0.961038

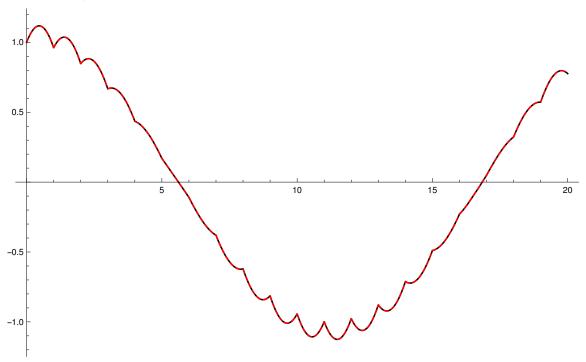
p1 = Plot[Re[phi1raw[x, Ceiling[x], 1, 1]], $\{x, 0, 20\}$, PlotStyle \rightarrow Black]



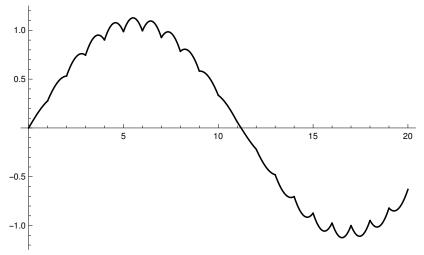
p2 = Plot[Re[phi2raw[x, Ceiling[x], 1, 1]], {x, 0, 20}, PlotStyle → {Red, Dashed}] (* same as Re(phi1raw) *)



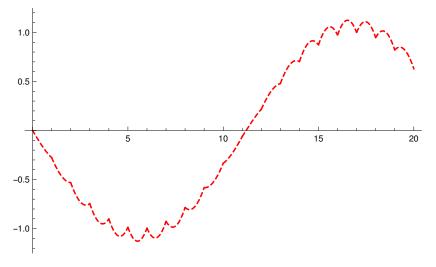




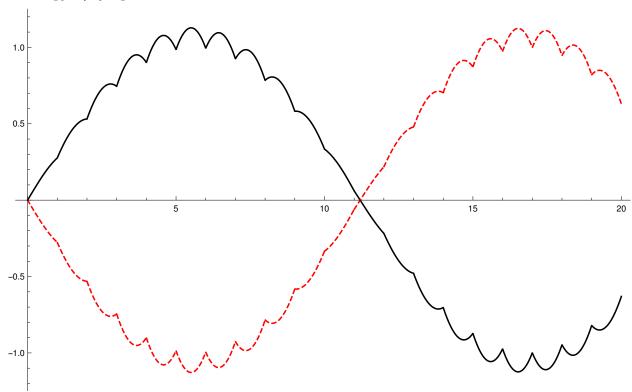
p3 = Plot[Im[phi1raw[x, Ceiling[x], 1, 1]], $\{x, 0, 20\}, PlotStyle \rightarrow Black]$



p4 = Plot[Im[phi2raw[x, Ceiling[x], 1, 1]], {x, 0, 20}, PlotStyle → {Red, Dashed}] (* -Im(phi1raw) *)



Show[p3, p4]



```
(* Show that phi1raw(x=n,n,q,epsilon) = Exp(i k n) *)
phi1raw[7, 7, 0.9, 0.2] // N
0.696237 - 0.717812 i
Exp[Ikk[0.9, 0.2]7] // N
0.696237 - 0.717812 i
phi1raw[8, 8, 2, 3] // N
-0.549437 - 0.835535 i
Exp[I kk[2, 3] 8] // N
-0.549437 - 0.835535 i
(* Show that phi2raw(x=n,n,q,epsilon) = Exp(-i k n) *)
phi2raw[7, 7, 0.9, 0.2] // N
0.696237 + 0.717812 i
Exp[-Ikk[0.9, 0.2] 7] // N
0.696237 + 0.717812 i
phi2raw[8, 8, 2, 3] // N
-0.549437 + 0.835535 i
Exp[-Ikk[2, 3] 8] // N
-0.549437 + 0.835535 i
```

```
(* Illustration: Geshkenbein Fig. 1 *)
f[k_{-}] := Cos[k] + epsilon / (2 k) Sin[k]
f[k]
Cos[k] + \frac{5 Sin[k]}{k}
plus[k_] := 1
minus[k_] := -1
epsilon:= 10
 (* value for v=epsilon used in Geshkenbein Fig. 1 *)
pp1 = Plot[{f[k], plus[k], minus[k]},
  \{k, 0, 19\}, PlotRange \rightarrow \{\{0, 19\}, \{-2, 2\}\},\
  PlotStyle → RGBColor[1, 0, 0]]
                                    10
```