

Task2_PeriodicMultilayer_Bandgap

May 17, 2016

```
In [3]: import numpy as np
import scipy as sp
import scipy.sparse.linalg as linalg
import matplotlib.pyplot as plt
%matplotlib inline
```

1 Task 2: 1D Periodic Multilayer Dielectric Slab, Eigenmode formulation

1.1 Maxwell Equations (time domain)

$$\nabla \times E = -\mu \frac{\partial H}{\partial t} \quad (1)$$

$$\nabla \times H = \epsilon \frac{\partial E}{\partial t} \quad (2)$$

1.2 Time Domain \rightarrow Frequency Domain

Using the Fourier transform we get:

$$E(r, t) \rightarrow E(r, \omega) \quad (3)$$

$$\frac{\partial E}{\partial t} \rightarrow i\omega E \quad (4)$$

Thus our wave equation transforms into:

$$\nabla E = -i\omega\mu H \quad (5)$$

$$\nabla E = -i\omega\epsilon E \quad (6)$$

1.3 1D Coordinates, Periodic

$$H_{yi}, E_{z_{i+\frac{1}{2}}}, i \in \mathcal{N} \quad (7)$$

$$H_{y0} = H_{yn} e^{ik_x a} \quad (8)$$

$$E_{z0+\frac{1}{2}} = E_{zn+\frac{1}{2}} e^{ik_x a} \quad (9)$$

$$\frac{\partial E_z}{\partial x} = -i\omega\mu H_y \quad (10)$$

$$\frac{\partial H_y}{\partial x} = i\omega\epsilon E_z \quad (11)$$

1.4 Discretization

$$\frac{\partial E_{zi}}{\partial x} \approx \frac{E_{zi+1} - E_{zi-1}}{\Delta x} \quad (12)$$

$$\frac{\partial E_{z0}}{\partial x} \approx \frac{E_{z1} - E_{zn} e^{ik_x a}}{\Delta x} \quad (13)$$

$$\frac{\partial E_{zn}}{\partial x} \approx \frac{E_{z0} e^{ik_x a} - E_{zn-1}}{\Delta x} \quad (14)$$

Forward difference

$$-i\omega\mu_i E_{zi+\frac{1}{2}} \approx \frac{H_{yi+1} - H_{yi}}{\Delta x} \quad (15)$$

Backward difference

$$-i\omega\epsilon_i H_{yi} \approx \frac{E_{zi+\frac{1}{2}} - E_{zi-\frac{1}{2}}}{\Delta x} \quad (16)$$

1.5 Wave equation

$$H_{yi} = \frac{i}{\omega\mu_i} \frac{\partial E_{zi}}{\partial x} \quad (17)$$

$$E_{zi} = \frac{-i}{\omega\epsilon_i} \frac{\partial H_{yi}}{\partial x} \quad (18)$$

$$\frac{\partial}{\partial x} \frac{i}{\omega\mu_i} \frac{\partial}{\partial x} E_{zi} = i\omega\epsilon_i E_{zi} \quad (19)$$

$$\frac{1}{\epsilon_i} \frac{\partial}{\partial x} \frac{1}{\mu_i} \frac{\partial}{\partial x} E_{zi} = \omega^2 E_{zi} \quad (20)$$

or

$$\frac{1}{\mu_i} \frac{\partial}{\partial x} \frac{1}{\epsilon_i} \frac{\partial}{\partial x} H_{yi} = \omega^2 H_{yi} \quad (21)$$

1.6 Matrix form

$$H_{y_i} = \frac{i}{\omega \mu_i} \frac{\partial E_z}{\partial x} \approx \frac{i}{\omega \mu_i} \frac{E_{z_{i+\frac{1}{2}}} - E_{z_{i-\frac{1}{2}}}}{\Delta x} \quad (22)$$

$$\begin{bmatrix} H_{y_0} \\ H_{y_1} \\ \vdots \\ H_{y_{n-1}} \\ H_{y_n} \end{bmatrix} = \frac{i}{\omega \Delta x} \begin{bmatrix} \frac{1}{\mu_0} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\mu_1} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\mu_2} & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & 0 & \frac{1}{\mu_n} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \dots & -e^{ik_x a} \\ -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & -1 & 1 \end{bmatrix} \begin{bmatrix} E_{z_{0+\frac{1}{2}}} \\ E_{z_{1+\frac{1}{2}}} \\ \vdots \\ E_{z_{n-\frac{1}{2}}} \\ E_{z_{n+\frac{1}{2}}} \end{bmatrix} \quad (23)$$

$$E_{z_{i+\frac{1}{2}}} = \frac{-i}{\omega \epsilon_i} \frac{\partial H_{y_i}}{\partial x} \approx \frac{-i}{\omega \epsilon_i} \frac{H_{y_{i+1}} - H_{y_i}}{\Delta x} \quad (24)$$

$$\begin{bmatrix} E_{z_{0+\frac{1}{2}}} \\ E_{z_{1+\frac{1}{2}}} \\ \vdots \\ E_{z_{n-\frac{1}{2}}} \\ E_{z_{n+\frac{1}{2}}} \end{bmatrix} = \frac{i}{\omega \Delta x} \begin{bmatrix} \frac{1}{\epsilon_0} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\epsilon_1} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\epsilon_2} & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & 0 & \frac{1}{\epsilon_n} \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ 0 & 0 & -1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 \\ e^{ik_x a} & 0 & \dots & 0 & -1 \end{bmatrix} \begin{bmatrix} H_{y_0} \\ H_{y_1} \\ \vdots \\ H_{y_{n-1}} \\ H_{y_n} \end{bmatrix} \quad (25)$$

$$\omega^2 E_z = \frac{1}{\epsilon} \frac{\partial}{\partial x} \frac{1}{\mu} \frac{\partial}{\partial x} E_z \quad (26)$$

$$\omega^2 \begin{bmatrix} E_{z_{0+\frac{1}{2}}} \\ E_{z_{1+\frac{1}{2}}} \\ \vdots \\ E_{z_{n-\frac{1}{2}}} \\ E_{z_{n+\frac{1}{2}}} \end{bmatrix} = \frac{i}{\Delta x} \begin{bmatrix} \frac{1}{\epsilon_0} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\epsilon_1} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\epsilon_2} & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & 0 & \frac{1}{\epsilon_n} \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ 0 & 0 & -1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 \\ e^{ik_x a} & 0 & \dots & 0 & -1 \end{bmatrix} \frac{i}{\Delta x} \begin{bmatrix} \frac{1}{\mu_0} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\mu_1} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\mu_2} & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & 0 & \frac{1}{\mu_n} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \\ \vdots & \vdots \\ 0 & 0 \end{bmatrix} \quad (27)$$

or, simplifying, and replacing $i + \frac{1}{2}$ with i :

$$\omega^2 \begin{bmatrix} E_{z_0} \\ E_{z_1} \\ \vdots \\ E_{z_{n-1}} \\ E_{z_n} \end{bmatrix} = -\frac{1}{\Delta x^2} \begin{bmatrix} \frac{1}{\epsilon_0} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\epsilon_1} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\epsilon_2} & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & 0 & \frac{1}{\epsilon_n} \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & \dots & 0 \\ 0 & 0 & -1 & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 1 \\ e^{ik_x a} & 0 & \dots & 0 & -1 \end{bmatrix} \begin{bmatrix} \frac{1}{\mu_0} & 0 & 0 & \dots & 0 \\ 0 & \frac{1}{\mu_1} & 0 & \dots & 0 \\ 0 & 0 & \frac{1}{\mu_2} & \dots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & 0 & \frac{1}{\mu_n} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \\ \vdots & \vdots & \vdots \\ 0 & 0 & \dots \end{bmatrix} \quad (28)$$

1.7 Boundary Conditions

In this case the boundary conditions are periodic, satisfied by the $e^{ik_x a}$ elements in the resulting matrix

2 Implementation

2.1 Setup grid

```
In [102]: n=200                # number of grid nodes

          dx=1/n                # discretization step, domain size = 1

          eps1 = 13              # Layer 1
          eps2 = 1              # Layer 2

          num_eigs = 6          # Solver for first # eigenmodes
```

2.2 Build matrix

```
In [103]: # Material parameters distribution

          eps = np.ones(n)
          eps[:int(n/2)-1] = 1/eps1
          eps[int(n/2):] = 1/eps2

          eps = sp.sparse.dia_matrix(([eps], [0]), [n,n])

          # Forward

          diag = np.ones(n) * -1/dx
          up_diag = np.ones(n) * 1/dx

          M_1 = sp.sparse.dia_matrix(([up_diag, diag], [1, 0]), [n,n])
          # Backward

          diag = np.ones(n) * 1/dx
          up_diag = np.ones(n) * -1/dx

          M_2 = sp.sparse.dia_matrix(([up_diag, diag], [-1, 0]), [n,n])

          M_1 = sp.sparse.lil_matrix(M_1)
          M_2 = sp.sparse.lil_matrix(M_2)
```

2.3 Solve for eigenmodes

```
In [117]: kk0 = 2*sp.pi*np.linspace(-0.5,0.5,300) # k-vector in medium with eps1-eps2

          k = np.zeros((num_eigs, kk0.size), dtype=complex)
          for ik in range(kk0.size):
              k0=kk0[ik]

          M_1[n-1, 0] = np.cos(k0*1)/dx # to impose periodic boundary condition
```

```

M_2[0, n-1] = -np.cos(k0*1)/dx

M = -eps*M_2*M_1

kt = k0/np.sqrt((eps1+eps2)/2); # target k=w/c
k2, V = linalg.eigs(M, k=num_eigs, M=None, sigma=kt**2)

k[:,ik] = np.sqrt(k2) # k=w/c

```

2.4 Plot eigenmodes

2.4.1 Bands

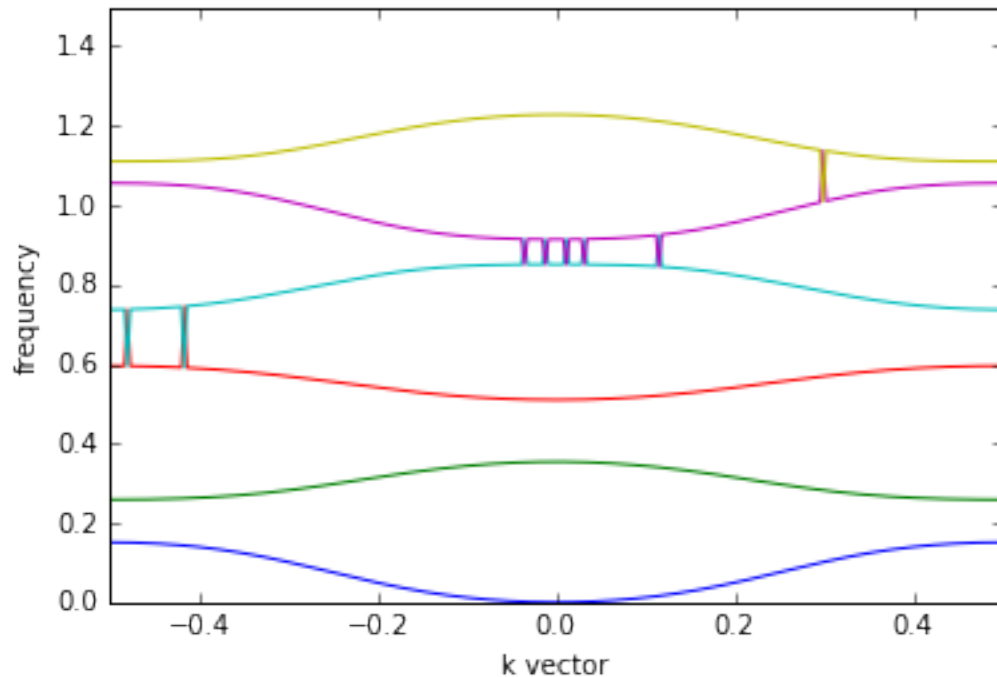
```

In [126]: for i in range(num_eigs):
            plt.hold(True)
            plt.plot(kk0/(2*sp.pi), np.real(k[i,:]/(2*sp.pi)) , '-')

plt.xlabel("k vector")
plt.ylabel("frequency")
plt.xlim([-0.5, 0.5])
plt.ylim([0.0, 1.5])

```

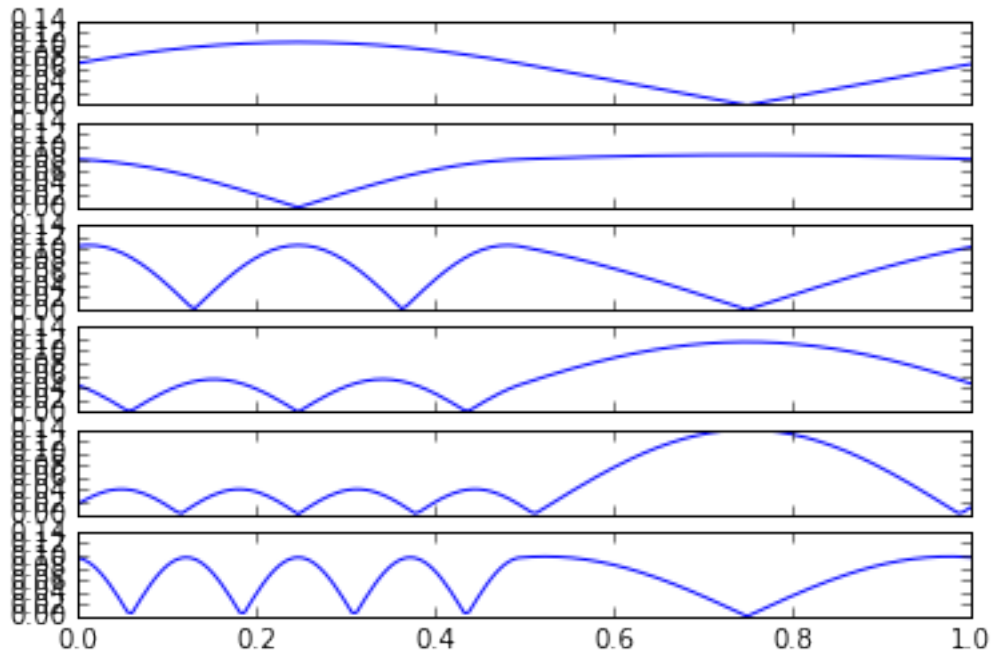
Out[126]: (0.0, 1.5)



2.4.2 Field distribution

```
In [119]: f, ax = plt.subplots(6,1, sharex=True, sharey=True)

for i in range(num_eigs):
    ax[i].plot(np.linspace(0, 1, n), np.abs(V[:,i]), '-')
```



2.5 Permittivity Contrast Bandgap dependence

```
In [128]: def build_bandgap_diagram(eps1, eps2, num_eigs=6):
    n=200                # number of grid nodes

    dx=1/n              # discretization step, domain size = 1

    # Material parameters distribution

    eps = np.ones(n)
    eps[:int(n/2)-1] = 1/eps1
    eps[int(n/2):] = 1/eps2

    eps = sp.sparse.dia_matrix(([eps], [0]), [n,n])

    # Forward

    diag = np.ones(n) * -1/dx
    up_diag = np.ones(n) * 1/dx
```

```

M_1 = sp.sparse.dia_matrix(([up_diag, diag], [1, 0]), [n,n])
# Backward

diag = np.ones(n) * 1/dx
up_diag = np.ones(n) * -1/dx

M_2 = sp.sparse.dia_matrix(([up_diag, diag], [-1, 0]), [n,n])

M_1 = sp.sparse.lil_matrix(M_1)
M_2 = sp.sparse.lil_matrix(M_2)

kk0 = 2*sp.pi*np.linspace(-0.5,0.5,300) # k-vector in medium with eps

k = np.zeros((num_eigs, kk0.size), dtype=complex)
for ik in range(kk0.size):
    k0=kk0[ik]

    M_1[n-1, 0] = np.cos(k0*1)/dx # to impose periodic boundary cond
    M_2[0, n-1] = -np.cos(k0*1)/dx

    M = -eps*M_2*M_1

    kt = k0/np.sqrt((eps1+eps2)/2); # target k=w/c
    k2, V = linalg.eigs(M, k=num_eigs, M=None, sigma=kt**2)

    k[:,ik] = np.sqrt(k2) # k=w/c

    return kk0/(2*sp.pi), np.real(k/(2*sp.pi))

```

2.5.1 $\epsilon_1 = 1, \epsilon_2 = 1$

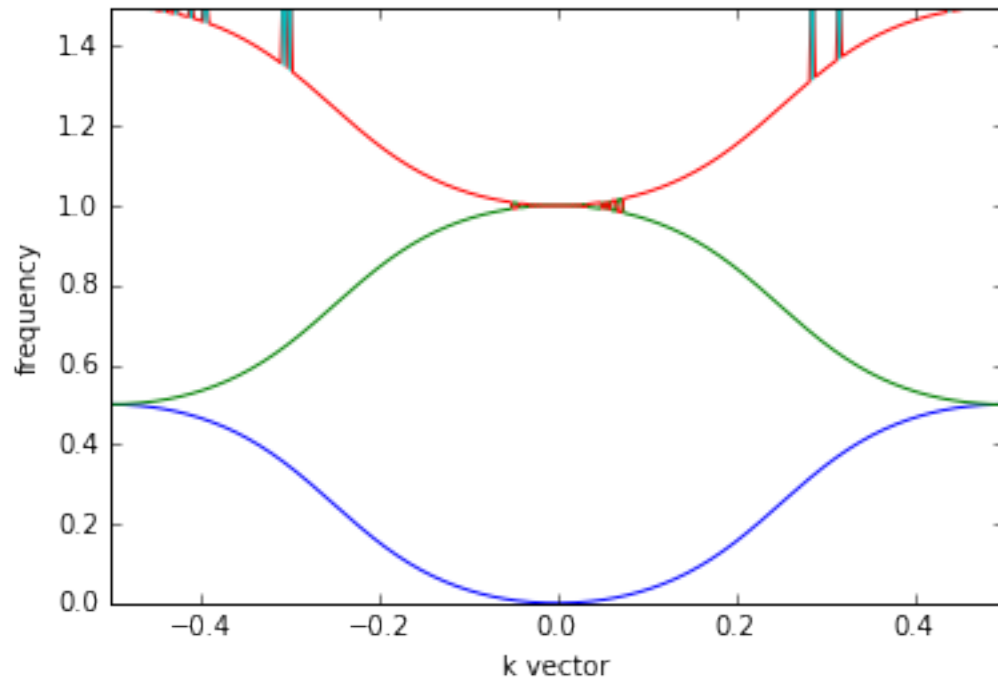
```

In [130]: k0, k = build_bandgap_diagram(1, 1, num_eigs)
          for i in range(num_eigs):
              plt.hold(True)
              plt.plot(k0, k[i,:], '-')

          plt.xlabel("k vector")
          plt.ylabel("frequency")
          plt.xlim([-0.5, 0.5])
          plt.ylim([0.0, 1.5])

```

Out[130]: (0.0, 1.5)

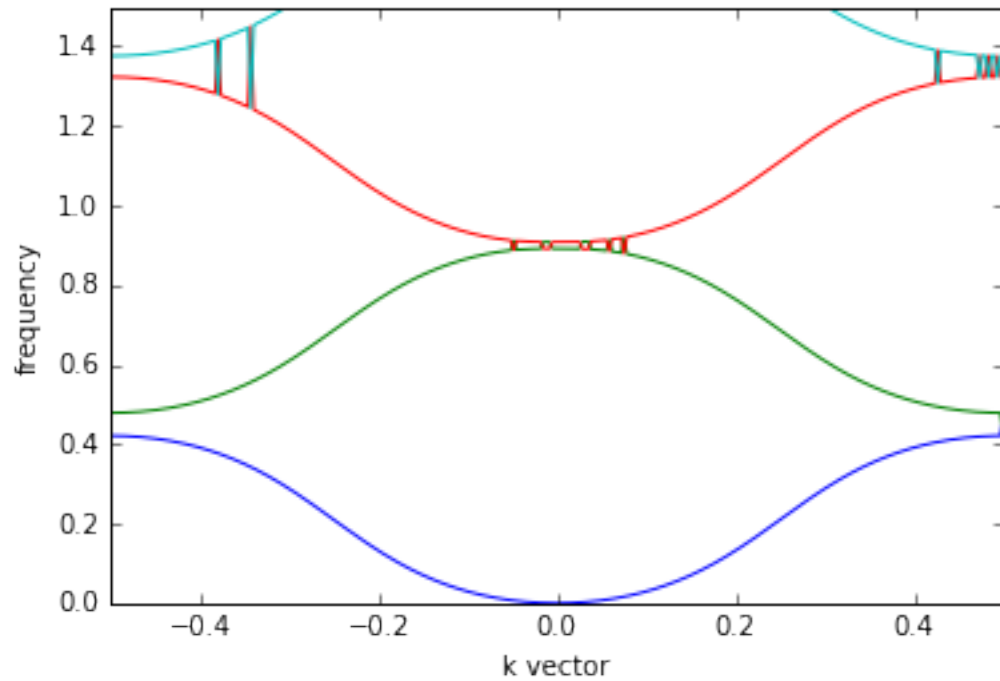


2.5.2 $\epsilon_1 = 1.5, \epsilon_2 = 1$

```
In [136]: k0, k = build_bandgap_diagram(1.5, 1, num_eigs)
           for i in range(num_eigs):
               plt.hold(True)
               plt.plot(k0, k[i,:], '-')

           plt.xlabel("k vector")
           plt.ylabel("frequency")
           plt.xlim([-0.5, 0.5])
           plt.ylim([0.0, 1.5])
```

```
Out[136]: (0.0, 1.5)
```

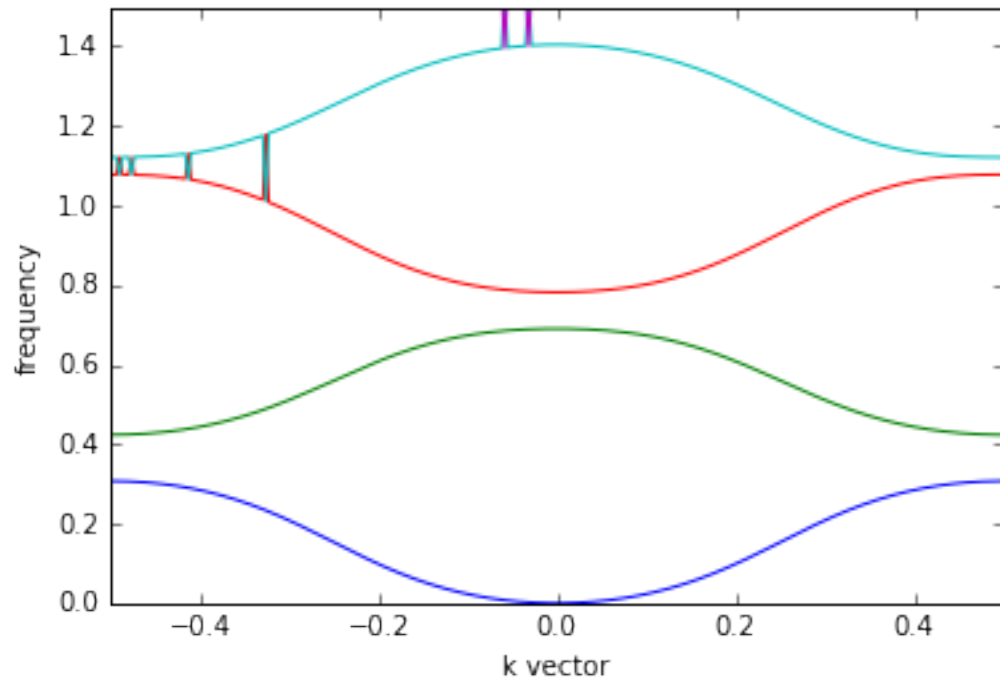



2.5.3 $\epsilon_1 = 3, \epsilon_2 = 1$

```
In [137]: k0, k = build_bandgap_diagram(3, 1, num_eigs)
          for i in range(num_eigs):
              plt.hold(True)
              plt.plot(k0, k[i, :], '-')

          plt.xlabel("k vector")
          plt.ylabel("frequency")
          plt.xlim([-0.5, 0.5])
          plt.ylim([0.0, 1.5])
```

Out[137]: (0.0, 1.5)

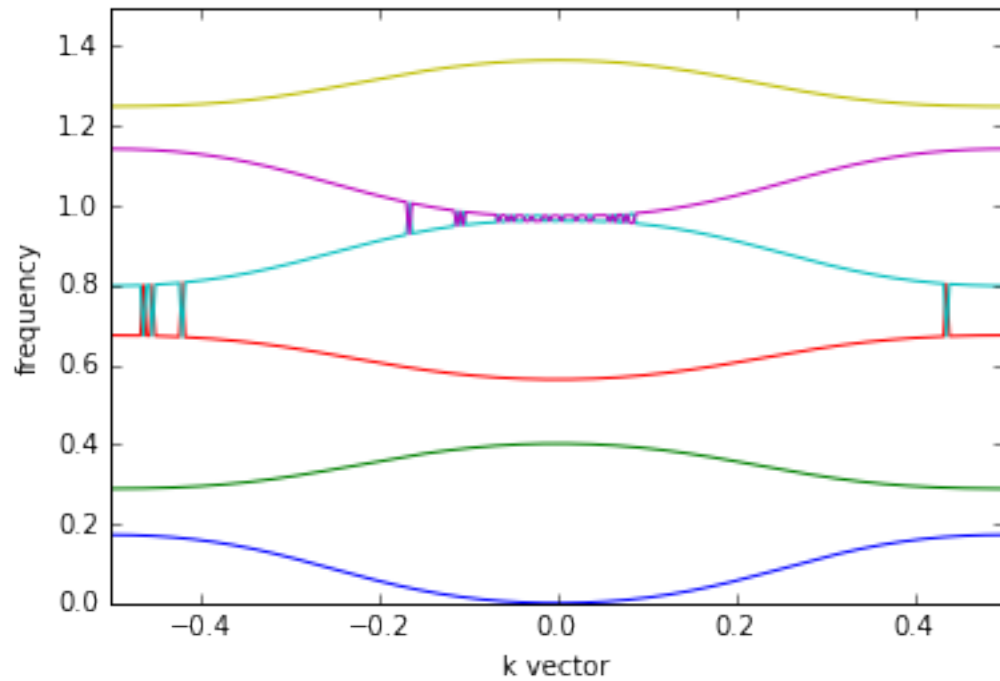


2.5.4 $\epsilon_1 = 10, \epsilon_2 = 1$

```
In [138]: k0, k = build_bandgap_diagram(10, 1, num_eigs)
           for i in range(num_eigs):
               plt.hold(True)
               plt.plot(k0, k[i, :], '-')

           plt.xlabel("k vector")
           plt.ylabel("frequency")
           plt.xlim([-0.5, 0.5])
           plt.ylim([0.0, 1.5])
```

Out[138]: (0.0, 1.5)

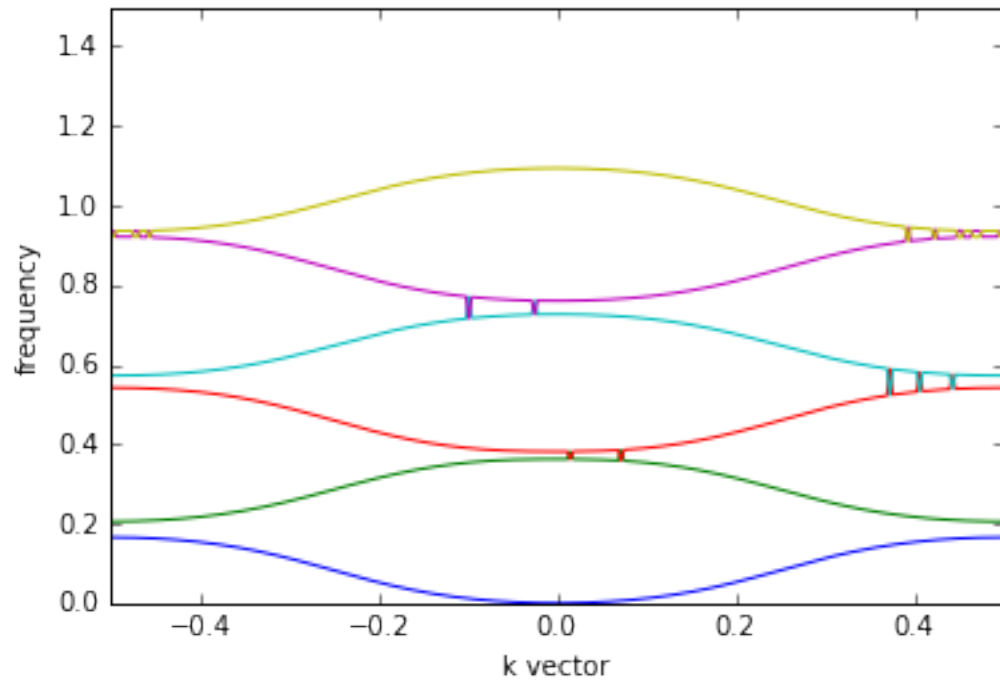


2.5.5 $\epsilon_1 = 10, \epsilon_2 = 5$

```
In [139]: k0, k = build_bandgap_diagram(10, 5, num_eigs)
          for i in range(num_eigs):
              plt.hold(True)
              plt.plot(k0, k[i, :], '-')

          plt.xlabel("k vector")
          plt.ylabel("frequency")
          plt.xlim([-0.5, 0.5])
          plt.ylim([0.0, 1.5])
```

Out[139]: (0.0, 1.5)

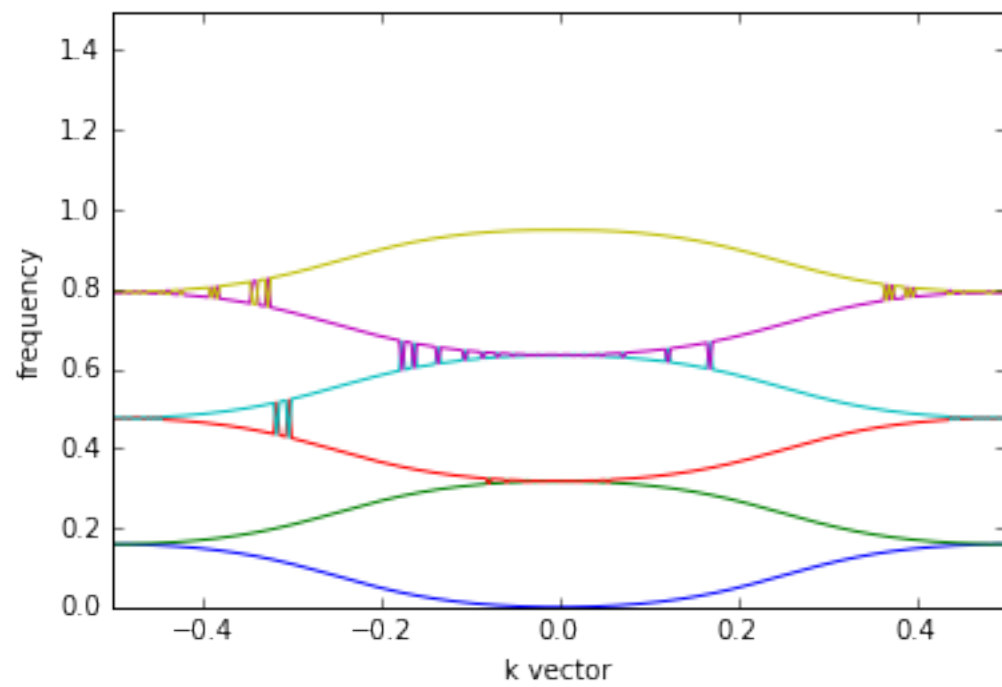


2.5.6 $\epsilon_1 = 10, \epsilon_2 = 10$

```
In [140]: k0, k = build_bandgap_diagram(10, 10, num_eigs)
          for i in range(num_eigs):
              plt.hold(True)
              plt.plot(k0, k[i,:], '-')

          plt.xlabel("k vector")
          plt.ylabel("frequency")
          plt.xlim([-0.5, 0.5])
          plt.ylim([0.0, 1.5])
```

```
Out[140]: (0.0, 1.5)
```



In []: