QSE 200 Sections

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CONTENTS

I am collecting notes/notebooks used in the QSE 200 (Fall 2022) Sections on this webpage.

CHAPTER

ONE

AN INTUITIVE PICTURE OF BAND STRUCTURE

I am following "Calculation of band structures by a discrete variable representation based on Bloch functions" (View online: https://doi.org/10.1119/1.1994858) to make a DVR method for periodic potentials.

```
import numpy as np
import matplotlib.pyplot as plt
```

1.1 Using the DVR scheme with periodic boundary conditions

```
hbar = 1
mu = 1

# Set these
M=100 # Basis size will be N=2M+1
P=5 # Periodicity

# Determined
xs = np.arange(0, P, P/(2*M+1))
```

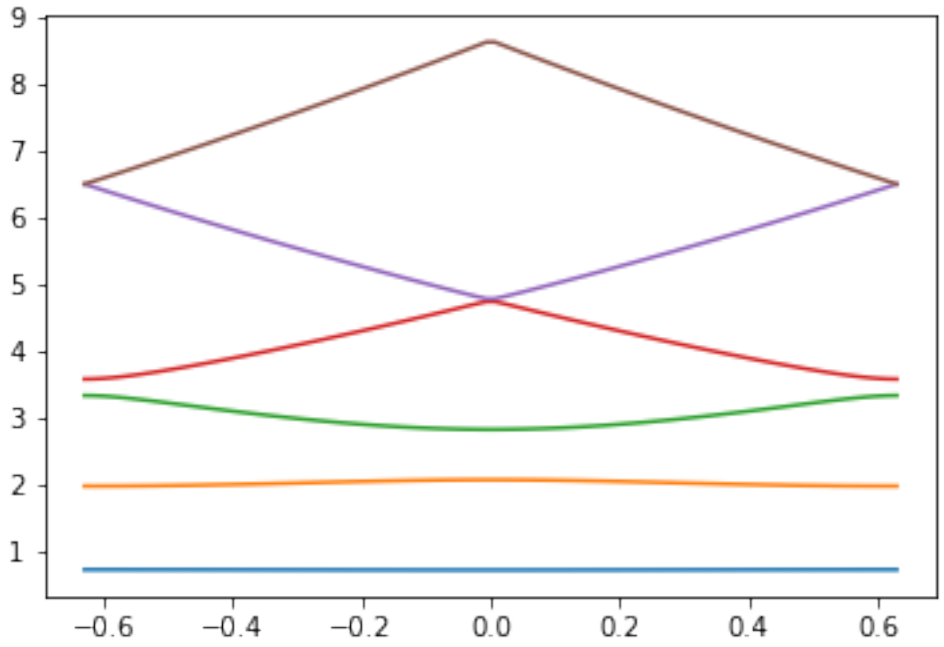
```
# Build the Hamiltonian
def make_H(kappa, P, M, Vfunc):
    N = 2*M+1
    Hmat = np.zeros((N,N), dtype=complex)
    Delta = P/N
    Delta_prime = np.pi/N
    omega = 2*np.pi/P
    for i in range(N):
        for j in range(N):
            if i==j:
                Hmat[i,j] = (hbar**2/(2*mu)) * (kappa**2 + omega**2 * (M*(M+1))/3) +␣
↪Vfunc(i*Delta)
            else:
                factor1 = (-1j*kappa*omega)/(np.sin((i-j)*Delta_prime))
                factor2 = omega**2 * np.cos((i-j)*Delta_prime)/(2*np.sin((i-j)*Delta_
↪prime)**2)
                Hmat[i,j] = (hbar**2/(2*mu)) * (-1)**(i-j) * np.exp(1j*kappa*(i-
↪j)*Delta) * (factor1+factor2)

    return Hmat
```

```
def Vfunc(x):
    return 1.5 + 1.5*np.cos(2*np.pi*x/P)
```

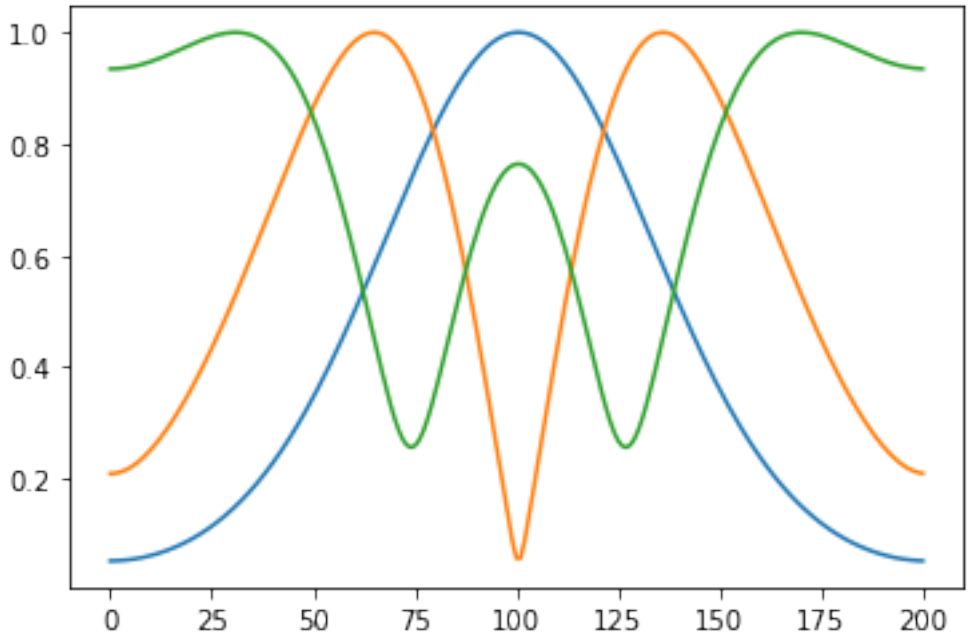
```
H=make_H(0.1, P, M, Vfunc)
vals, vecs = np.linalg.eigh(H)
```

```
kappa_vals= np.linspace(-np.pi/P,np.pi/P,100)
bands = np.zeros((6,len(kappa_vals)))
for (nk,kappa) in enumerate(kappa_vals):
    Hmat = make_H(kappa, P, M, Vfunc)
    vals, vecs = np.linalg.eigh(Hmat)
    bands[:,nk] = vals[0:6]
```

```
for band_val in range(6):
    plt.plot(kappa_vals, bands[band_val,:])
```



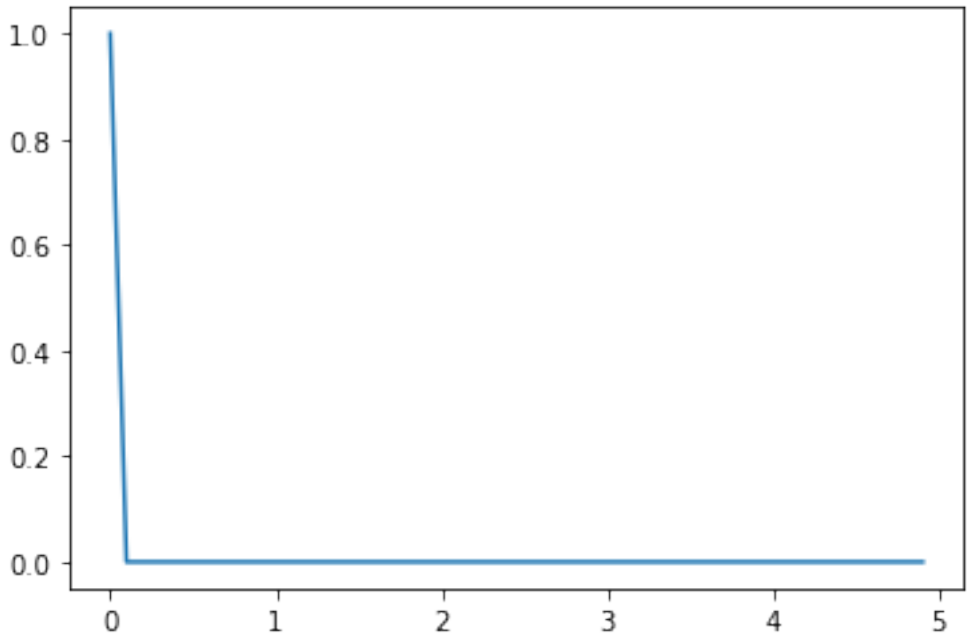

```
vals, vecs = np.linalg.eigh(make_H(0.2, P, M, Vfunc))
for i in range(3):
    plt.plot(np.abs(vecs[:,i])/np.max(np.abs(vecs[:,i])));
```



Now let's try more interesting unit cells. Start with the Kronig-Penney model.

```
def Vfunc(x):
    return 3*((np.abs(x) < P/4)|(np.abs(x)>3*P/4))

plt.plot(xs,Vfunc(xs))
```

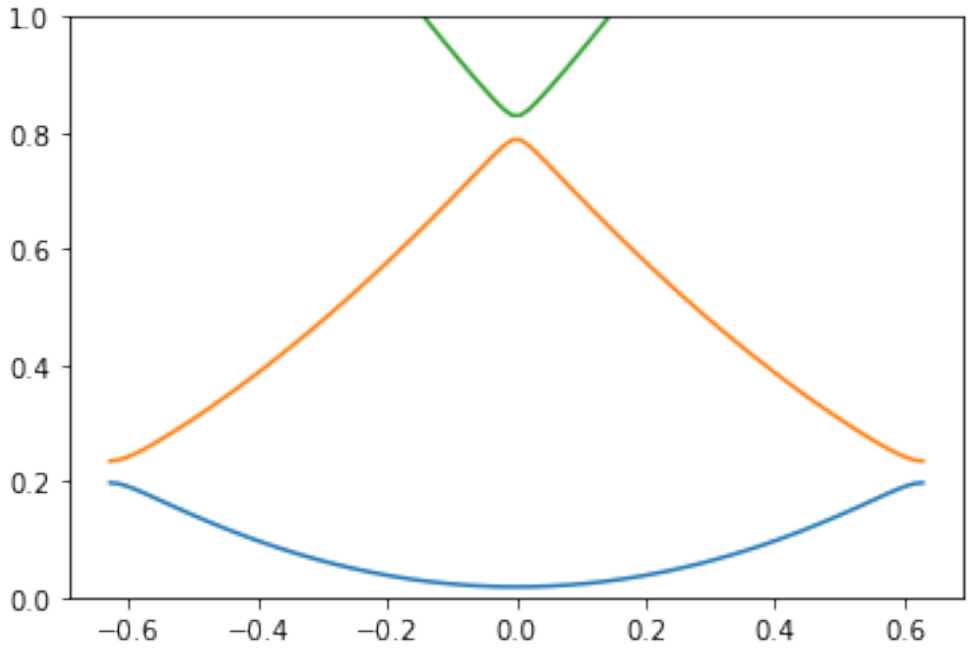
```
[<matplotlib.lines.Line2D at 0x7faa1b7a8220>]
```



```
kappa_vals= np.linspace(-np.pi/P,np.pi/P,100)
bands = np.zeros((6,len(kappa_vals)))
for (nk,kappa) in enumerate(kappa_vals):
    Hmat = make_H(kappa, P, M, Vfunc)
    vals, vecs = np.linalg.eigh(Hmat)
    bands[:,nk] = vals[0:6]
```

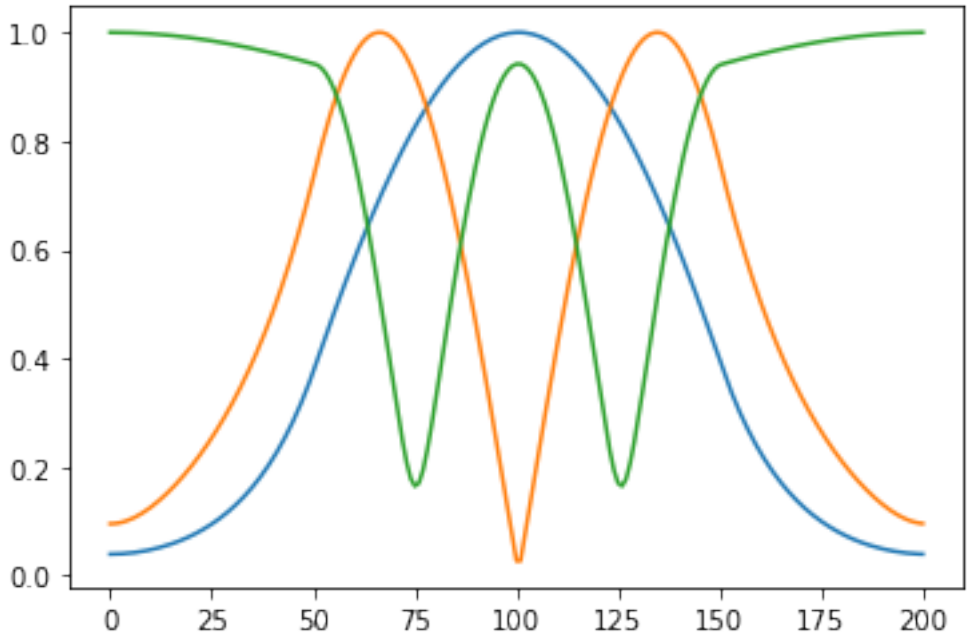
```
for band_val in range(6):
    plt.plot(kappa_vals, bands[band_val,:])
```

```
(0.0, 1.0)
```



Also plot the wavefunctions

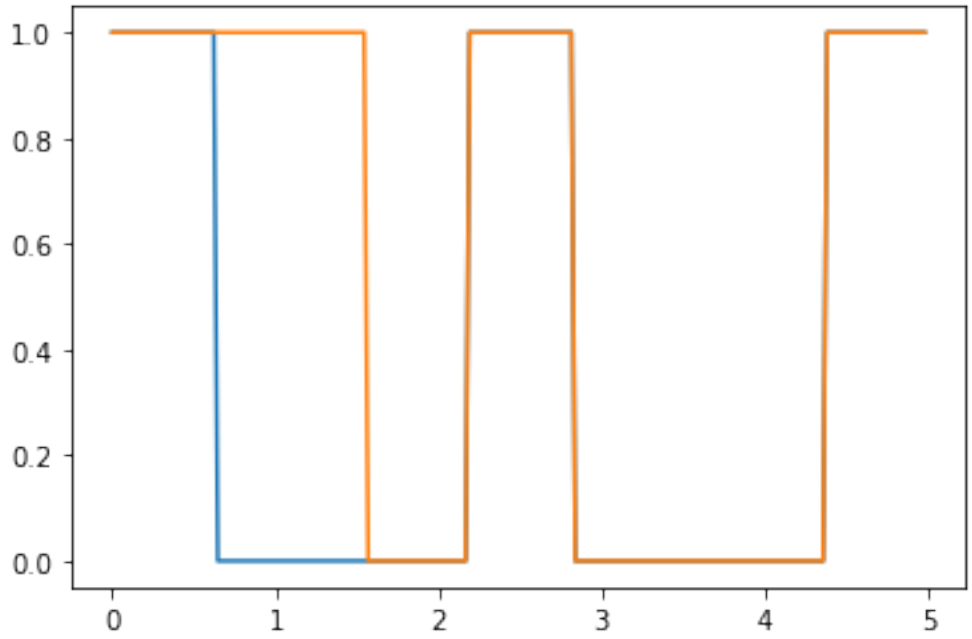
```
vals, vecs = np.linalg.eigh(make_H(0.2, P, M, Vfunc))
for i in range(3):
    plt.plot(np.abs(vecs[:,i])/np.max(np.abs(vecs[:,i])));
```



Try the double-well potential that Federico mentioned.

```
def Vfunc_sym(x):
    return -1+ 1*((np.abs(x) < P/8)|(np.abs(x)>3.5*P/8)) + 1*((np.abs(x) < 4.5*P/
 ↪8)|(np.abs(x)>7*P/8))

def Vfunc_asym(x):
    return -1+ 1*((np.abs(x) < 2.5*P/8)|(np.abs(x)>3.5*P/8)) + 1*((np.abs(x) < 4.5*P/
 ↪8)|(np.abs(x)>7*P/8))

plt.plot(xs,Vfunc_sym(xs))
plt.plot(xs,Vfunc_asym(xs))
```

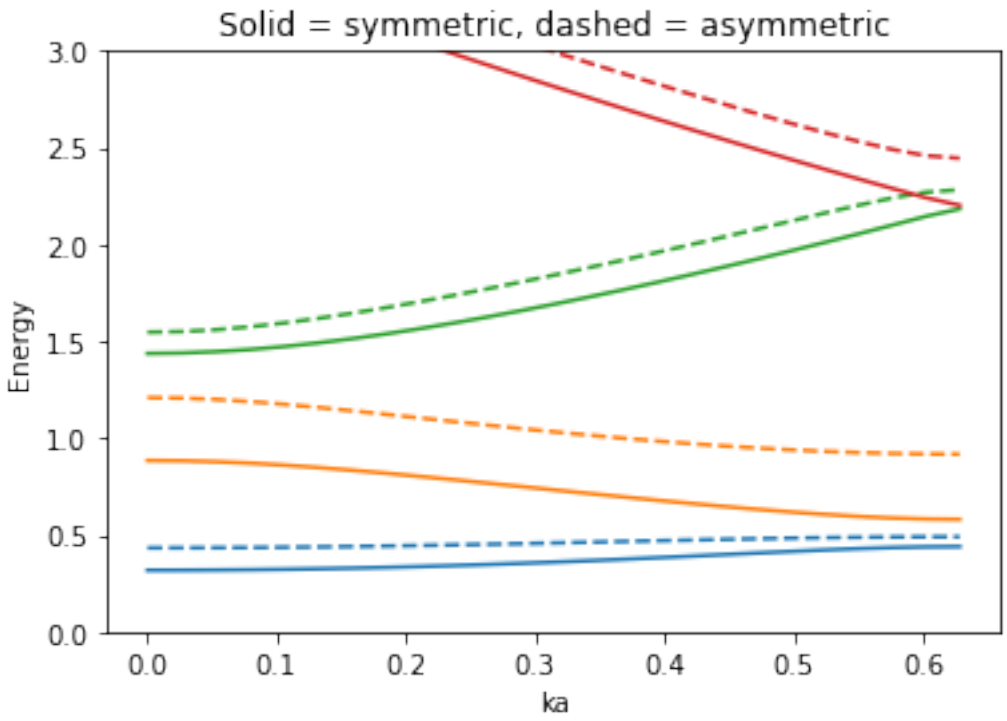
```
[<matplotlib.lines.Line2D at 0x7fb458d60670>]
```




```
kappa_vals= np.linspace(0,np.pi/P,25)
bands_sym = np.zeros((6,len(kappa_vals)))
for (nk,kappa) in enumerate(kappa_vals):
    Hmat = make_H(kappa, P, M, Vfunc_sym)
    vals, vecs = np.linalg.eigh(Hmat)
    bands_sym[:,nk] = vals[0:6]

kappa_vals= np.linspace(0,np.pi/P,25)
bands_asym = np.zeros((6,len(kappa_vals)))
for (nk,kappa) in enumerate(kappa_vals):
    Hmat = make_H(kappa, P, M, Vfunc_asym)
    vals, vecs = np.linalg.eigh(Hmat)
    bands_asym[:,nk] = vals[0:6]
```

```
colors = plt.rcParams['axes.prop_cycle'].by_key()['color']
for band_val in range(6):
    plt.plot(kappa_vals, bands_sym[band_val,:], color=colors[band_val])
    plt.plot(kappa_vals, bands_asym[band_val,:],'--', color=colors[band_val])
    plt.gca().set_prop_cycle(None)
plt.ylim(0,3)
plt.xlabel("ka")
plt.ylabel("Energy")
plt.title("Solid = symmetric, dashed = asymmetric")
```

```
Text(0.5, 1.0, 'Solid = symmetric, dashed = asymmetric')
```

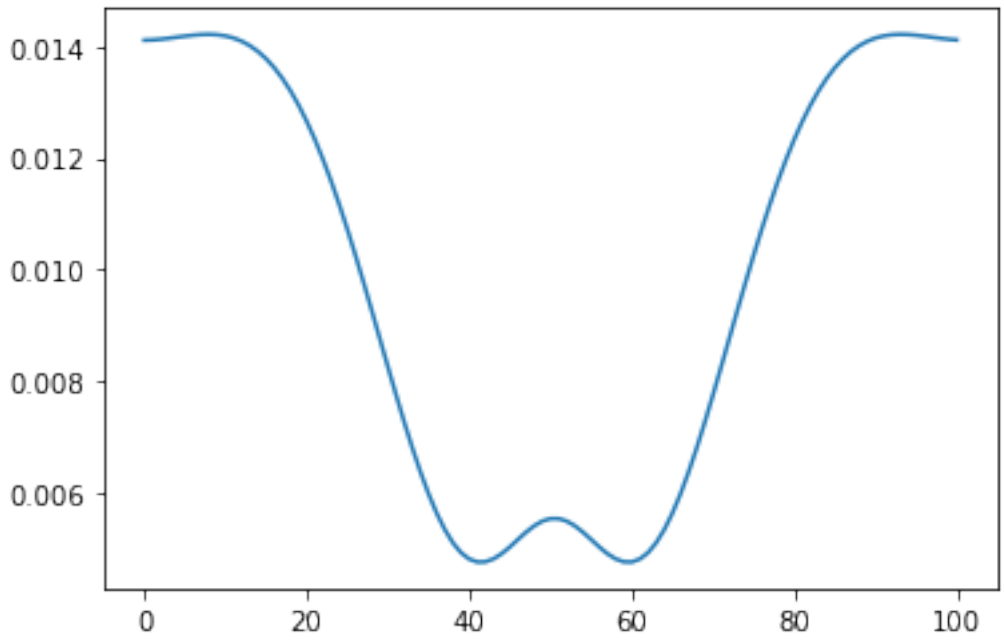


Also plot the wavefunctions for a particular kappa value

```
vals, vecs = np.linalg.eigh(make_H(0.352, P, M, Vfunc_sym))
```

```
plt.plot(np.abs(vecs[:,2])**2)
```

```
[<matplotlib.lines.Line2D at 0x7fb468adddc0>]
```

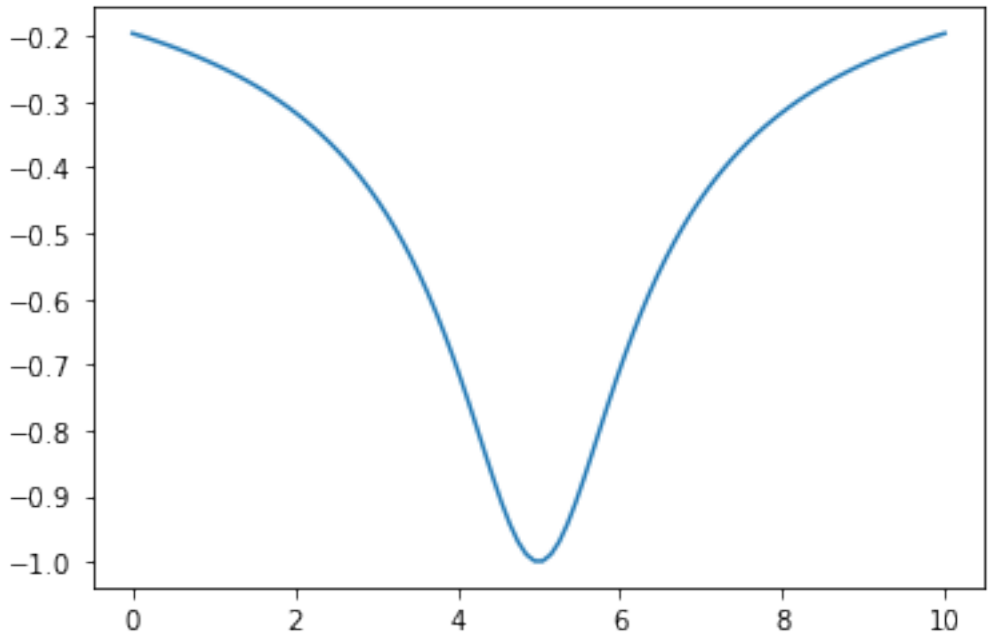


And the “soft Coulomb” potential

```
def V_C(x):
    return -1**2/np.sqrt(1**2+(x-10/2)**2)
```

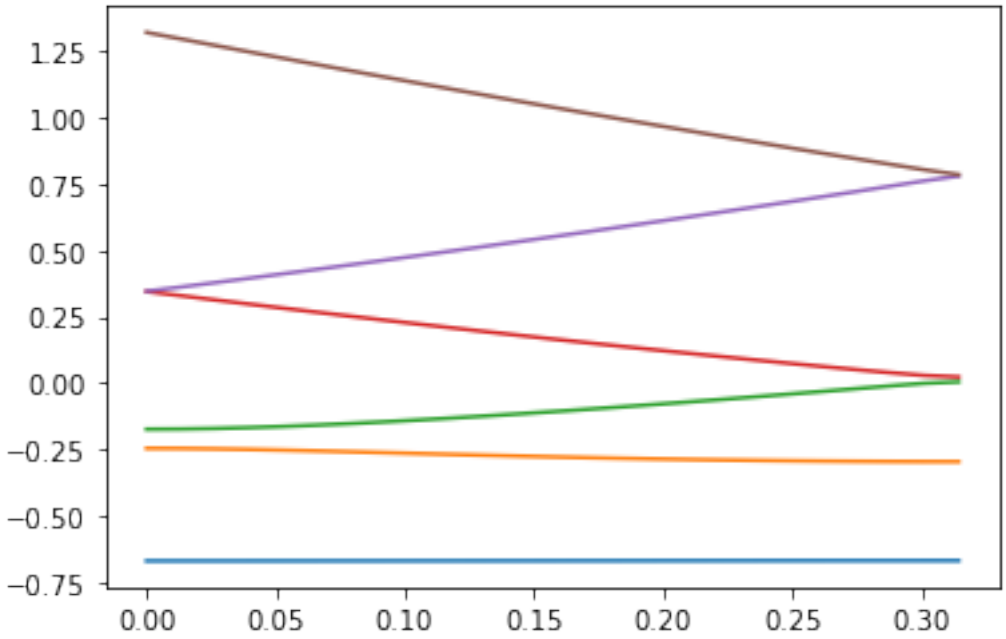
```
xs = np.linspace(0,10,100)
plt.plot(xs,V_C(xs))
```

```
[<matplotlib.lines.Line2D at 0x7fb47ab80fd0>]
```




```
P = 10
M = 50
kappa_vals= np.linspace(0,np.pi/P,25)
bands = np.zeros((6,len(kappa_vals)))
for (nk,kappa) in enumerate(kappa_vals):
    Hmat = make_H(kappa, P, M, V_C)
    vals, vecs = np.linalg.eigh(Hmat)
    bands[:,nk] = vals[0:6]
```

```
for band_val in range(6):
    plt.plot(kappa_vals, bands[band_val,:])
```

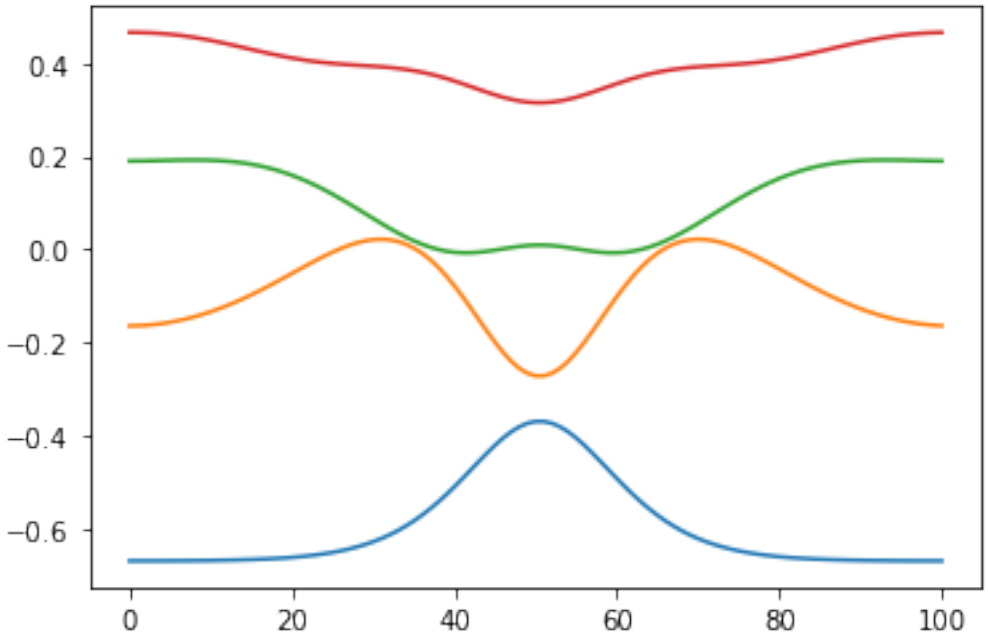



```
bands[0:4,[0,-1]]
```

```
array([[-0.67028101, -0.66929123],
       [-0.24614924, -0.29620133],
       [-0.17392269,  0.00475342],
       [ 0.34513722,  0.02303324]])
```

```
vals, vecs = np.linalg.eigh(make_H(0.157, P, M, V_C))
```

```
for i in range(4):
    plt.plot(vals[i]+0.3*np.abs(vecs[:,i])**2/np.max(np.abs(vecs[:,i])**2))
```



1.2 Also try the sinc-basis DVR code and program some "periodic" potentials by hand

```
hbar = 1
m = 1
```

```
# Function to make the kinetic energy operator
def make_T(x):
    Delta_x = x[1]-x[0]
    N = x.shape[0]
    Tmat = np.zeros((N,N))

    # now loop over kinetic energy matrix and fill in matrix elements
    for i in range(N):
        for j in range(N):
            if i==j:
                Tmat[i,j] = (hbar**2/(2*m*Delta_x**2)) * (np.pi**2)/3
            else:
                Tmat[i,j] = (hbar**2/(2*m*Delta_x**2)) * (-1)**(i-j) * 2/(i-j)**2

    return Tmat

# Function to make the potential energy operator
def make_V(x,Vfunc):
    Vmat = np.zeros((len(x),len(x)))
    for i in range(len(x)):
        Vmat[i,i] = Vfunc(x[i])
    return Vmat

# Function to make the full Hamiltonian
```

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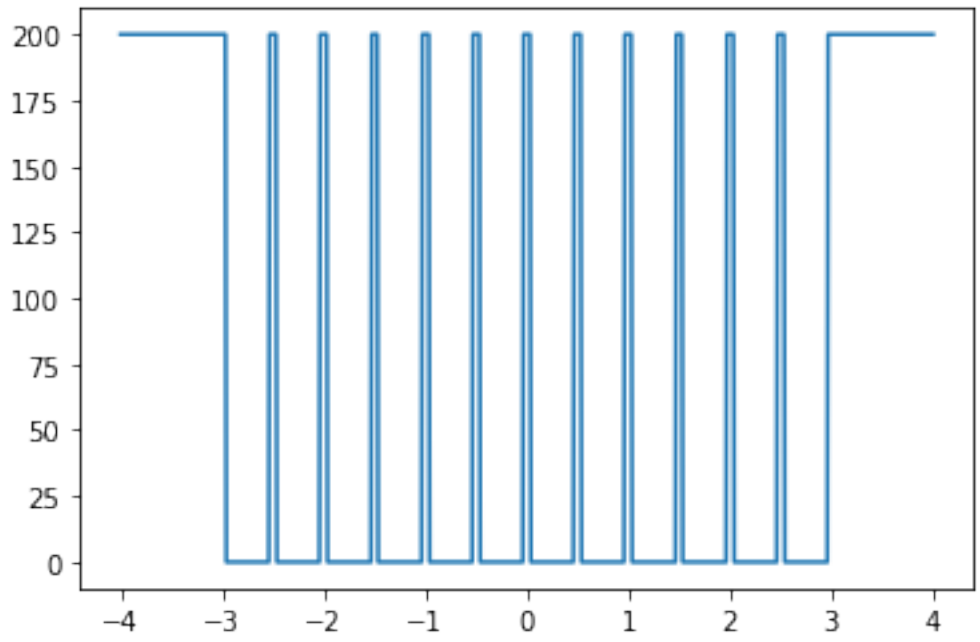
```
def make_H(x,Vfunc):
    return make_T(x) + make_V(x,Vfunc)
```

```
N = 900
xs = np.linspace(-4,4,N)
```

```
def V_wells(x):
    out = 0
    if np.abs(x) > 3.0:
        out += 200
    else:
        for n in range(-10,10):
            if ((x-0.035) < 0.5*n)&((x+0.035)>0.5*n):
                out += 200
    return out
```

```
plt.plot(xs,[V_wells(xs[i]) for i in range(len(xs))])
```

```
[<matplotlib.lines.Line2D at 0x7faa1c7b0e50>]
```

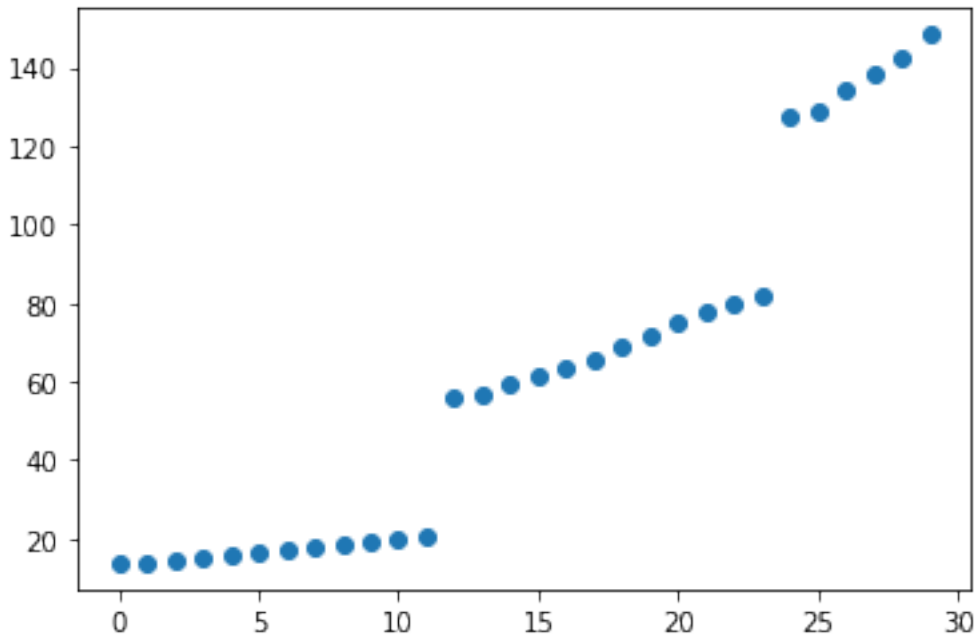



```
Ham=make_H(xs,V_wells)
```

```
vals, vecs = np.linalg.eigh(Ham)
```

```
plt.plot(vals[0:30],'o')
```

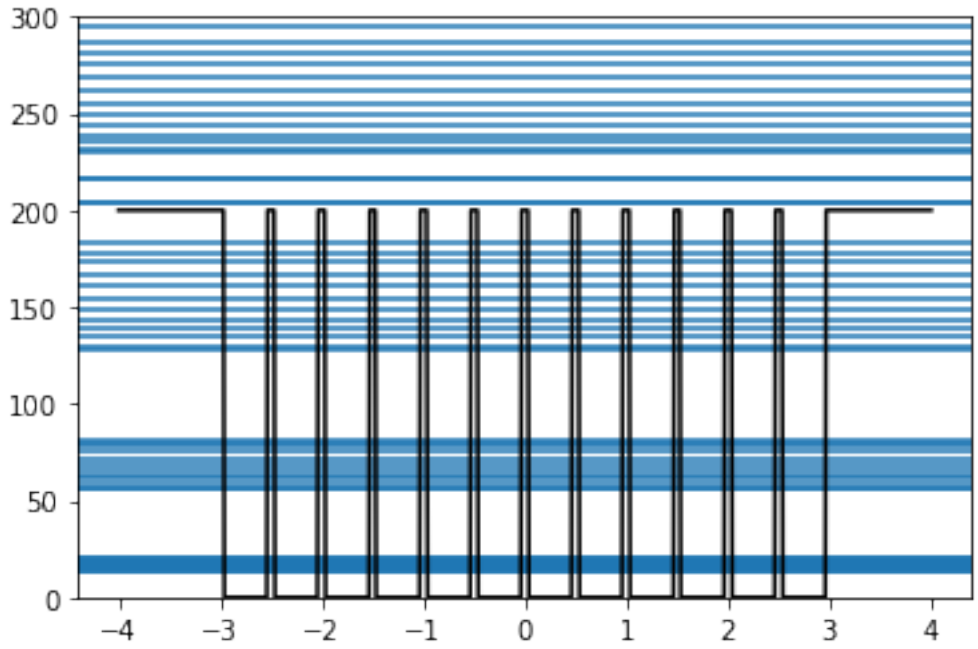
```
[<matplotlib.lines.Line2D at 0x7faa2a84f8b0>]
```




```
for i in range(100):
    plt.axhline(vals[i])

plt.plot(xs,[V_wells(xs[i]) for i in range(len(xs))],'k')
plt.ylim(0,300)
```

```
(0.0, 300.0)
```



1.3 Use transfer matrix approach

```
m =1
```

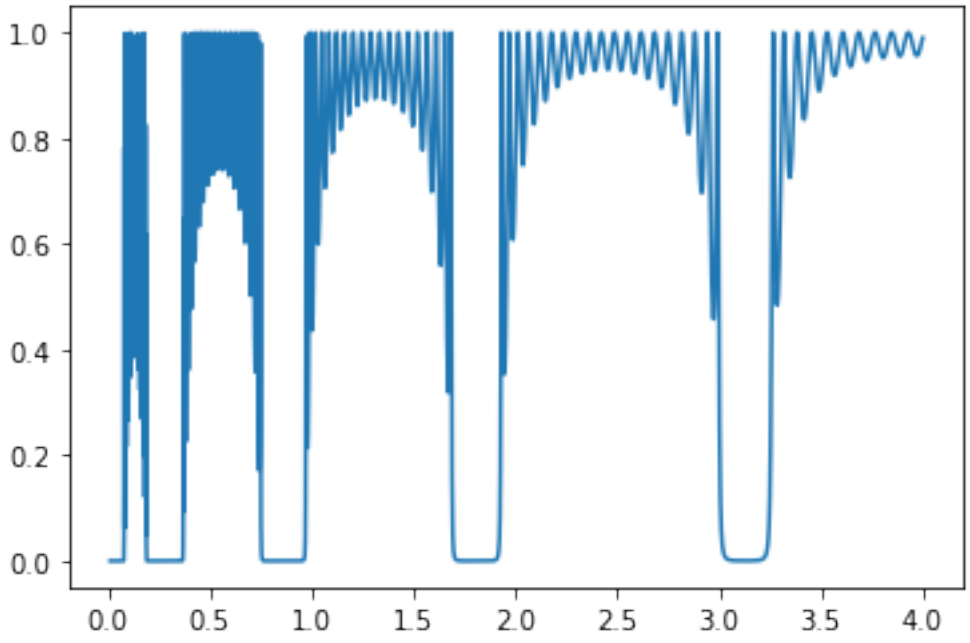
```
def DMat(k1, k2):
    res = np.zeros((2,2),dtype=np.complex_)
    res[0,0] = (1 + k2/k1)/2
    res[0,1] = (1 - k2/k1)/2
    res[1,0] = res[0,1]
    res[1,1] = res[0,0]
    return res

def PMat(k, L):
    res = np.zeros((2,2),dtype=np.complex_)
    res[0,0] = np.exp(-1j * k * L)
    res[1,1] = np.exp(1j * k * L)
    return res
```

```
Es = np.arange(0.01, 4.0, 0.0005) #1.6
width_barrier = 0.12
width_gap = 5
Ttrans = np.zeros(Es.size)
i = 0
for E in Es:
    klow = np.emath.sqrt(2 * m * E)
    khigh = np.emath.sqrt(2 * m * (E - Vb))
    res_mat = DMat(klow, khigh) @ PMat(khigh, width_barrier) @ DMat(khigh, klow) @␣
 ↪PMat(klow, width_gap)
    U, V = np.linalg.eig(res_mat)
    diag_res_mat = np.diag([U[0],U[1]])
    res_mat = np.linalg.matrix_power(diag_res_mat,20)
    res_mat = V @ res_mat @ np.linalg.inv(V)
    Ttrans[i] = 1 - np.abs(res_mat[1, 0])**2 / np.abs(res_mat[0,0])**2
    i = i + 1

plt.plot(Es, Ttrans)
```

```
[<matplotlib.lines.Line2D at 0x7fe5147d8670>]
```


1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0

CHAPTER

TWO

TRANSLATION OPERATORS AND BLOCH'S THEOREM

CHAPTER

THREE

THE KRONIG-PENNEY MODEL

The Kronig-Penney model is a simple model of electrons moving in a 1D potential. It is very reminiscent of the approach we took in *Section 6*, although allows us to look at the problem analytically. The approach is as follows: consider the Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{3.1}$$

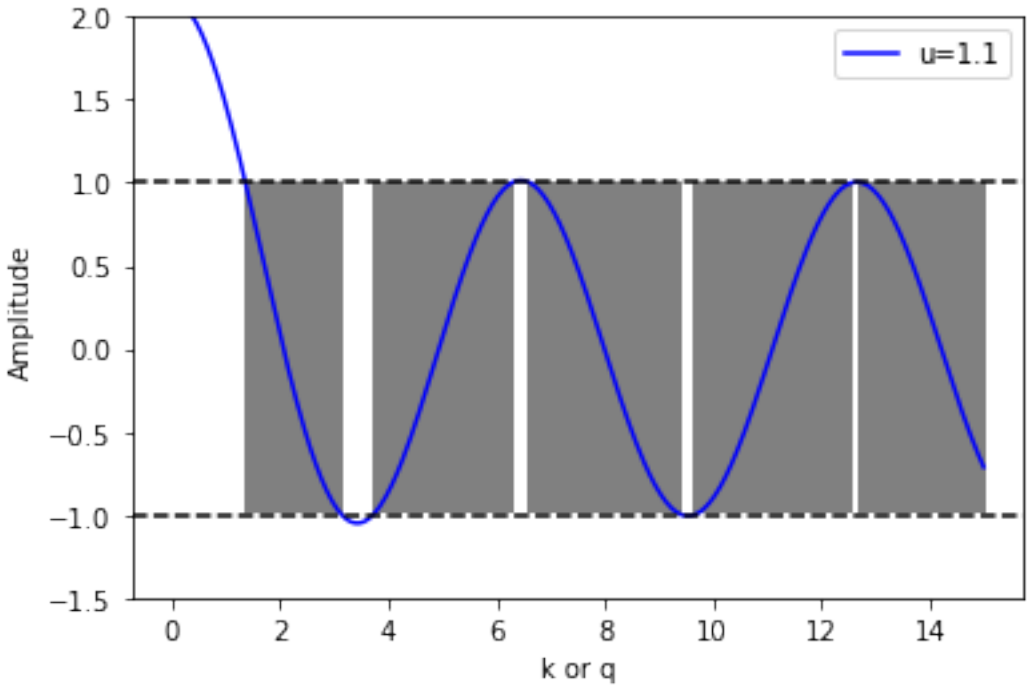
where $ V(x) $ is the potential due to a series of Delta functions that are evenly spaced and all have the same strength.

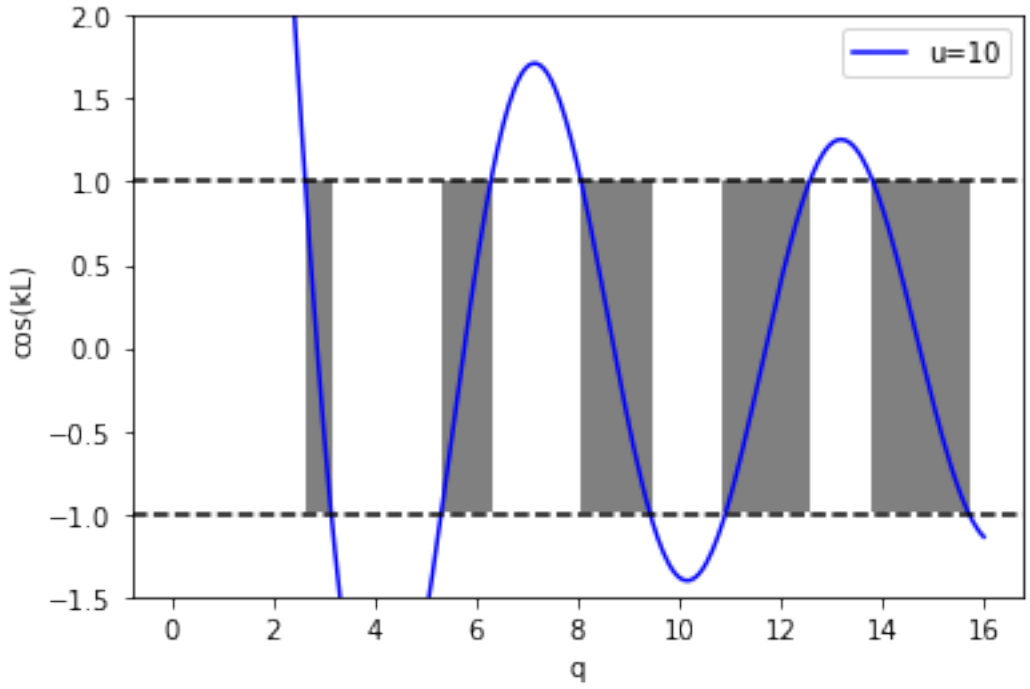
The solutions must satisfy

$$\cos(qa) = \cos(ka) + u\frac{\sin(ka)}{ka}. \tag{3.2}$$

The left-hand side is clearly restricted $[-1,1]$ while the right-hand side is not. For the values of k that make the right-hand side have magnitude greater than 1, there will be no allowed energy eigenstates—there will be gaps in the energy spectrum. On the other hand, when k takes a value such that the right-hand side has magnitude less than 1, there will be a valid solution and allowed energy eigenstates—this leads to the formation of energy bands over the range of permissible k values.

To investigate this, let's look at the equation graphically. Since the left-hand side of *(3.2)* is always in the range $[-1,1]$, we'll draw two horizontal lines at ±1. We can then plot the right-hand side for a few different values of u and look at where this falls in the range that solutions exist.






```
/var/folders/xx/v9dchmf97dd5b8x7jswjw5yc0000gn/T/ipykernel_53640/4063795205.py:28:␣
↪RuntimeWarning: invalid value encountered in arccos
  qsolve.append(np.arccos(np.cos(q[i])+u*np.sin(q[i])/q[i]))
```

```
plt.plot(qsolve,ksolve)
```

```
[<matplotlib.lines.Line2D at 0x7fd764580700>]
```