Semiconductor Bloch Equations with Coulomb Interaction

Abstract

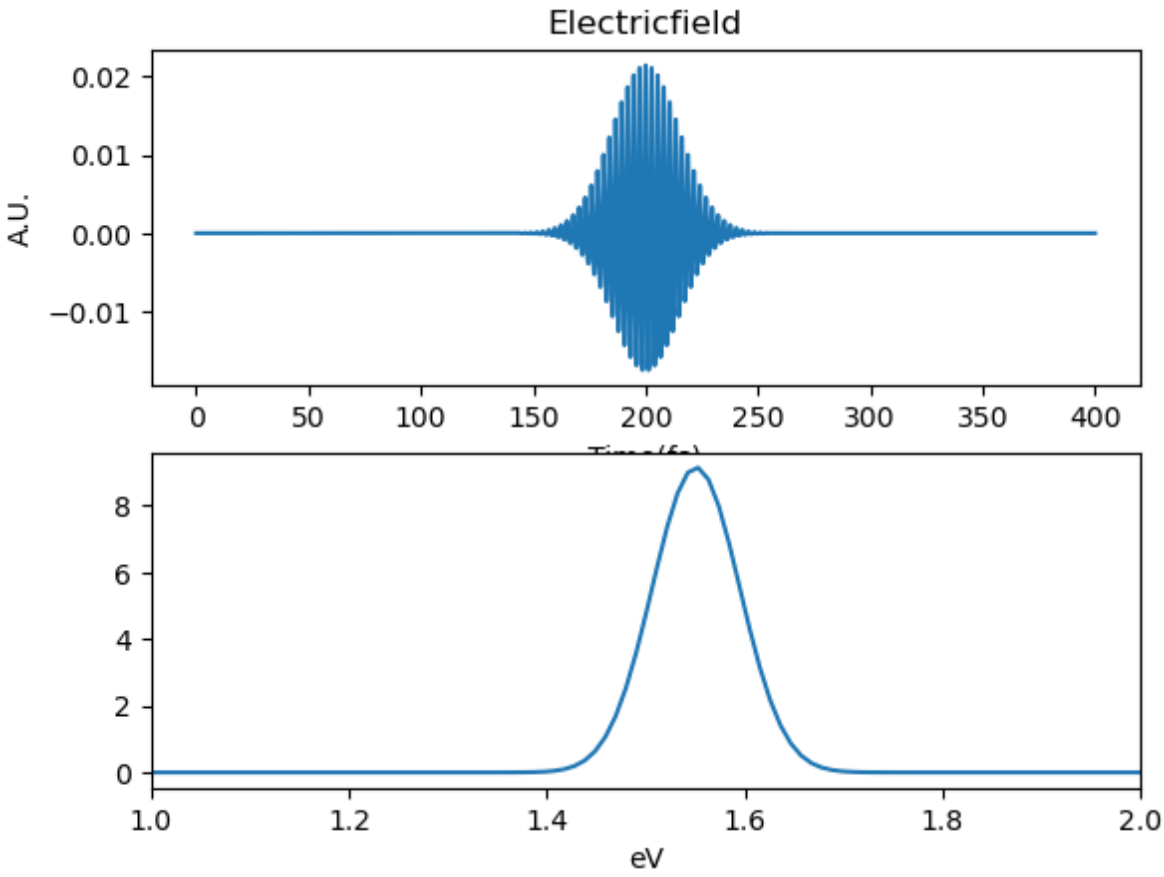
This python module **SBEwithCI.py** is developed for simulating exciton effect on optical response in solid with Semiconductor Bloch Equations (SBEs).

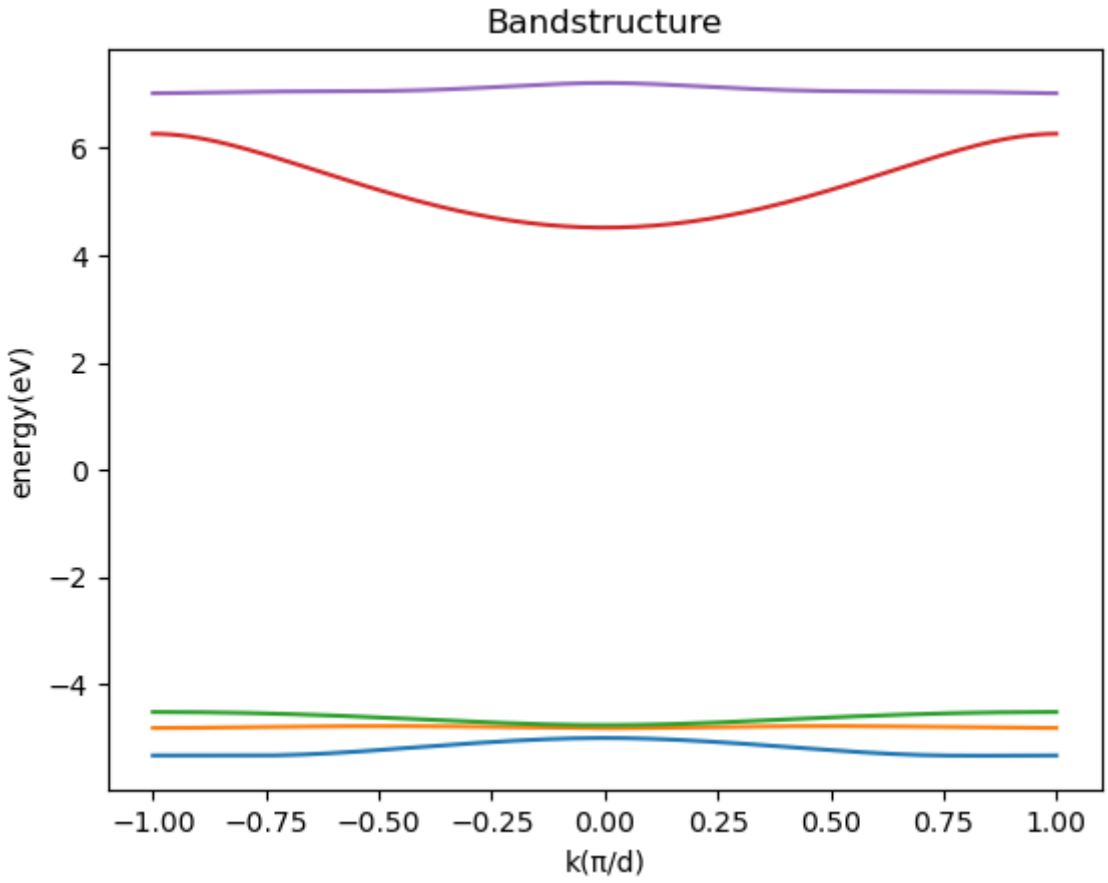
Quick Start

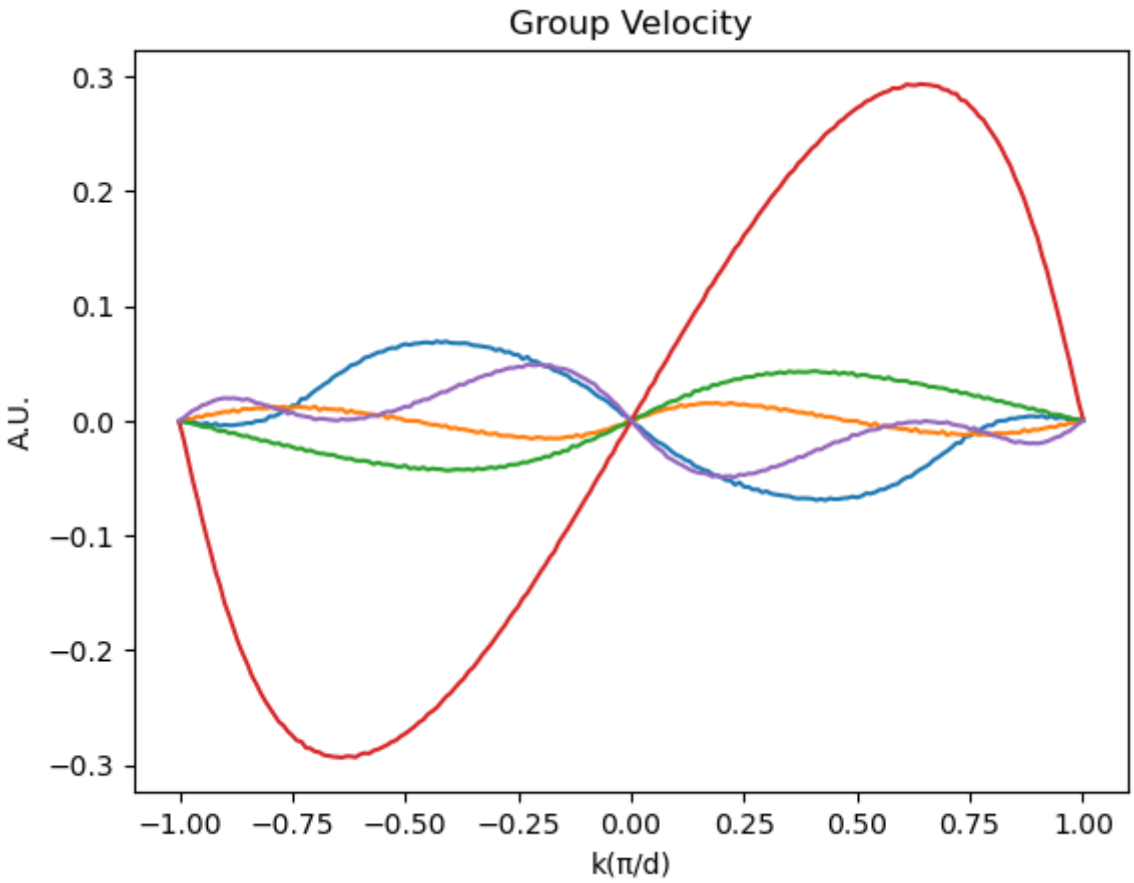
run test.py

In [1]:
```
import numpy as np
import scipy
from matplotlib import pyplot as plt
from math import sqrt
from SBEwithCI import SBE, loadband, Matplot
import time as tp
import copy
from multiprocessing import Pool
import multiprocessing as mp
from matplotlib import cm

from numpy.fft import fft, fftfreq,fftshift,ifft

#all the value should be convert to atomic unit

if __name__ == '__main__': #similar to main function in C/C++, multiprocessing need


    pi=scipy.constants.pi #pi constant
    d=9.32                  #lattice constant
    t=np.linspace(0,41*400,10000) #time axis
    k=np.linspace(-pi/d, pi/d,201)    #k axis
    dk=k[1]-k[0]


    #set electric field 0
    w1=0.057       #frequency
    tau=41*25*sqrt(2) #pulse duration
    fi=0               #phase
    E0=1e10             #field strength
    E0field=np.exp(-4*np.log(2)*((t-41*200)/tau)**2)*np.cos(w1*(t-41*200)+fi)/5.14

    #set electric field 1 (optional)
    w2=0.057*2         #frequency
    tau1=41*30*sqrt(2) #pulse duration
    fi1=0             #phase
    E1=1e9          #field strength
    delay=0          #delay between two pulses
    E1field=np.exp(-4*np.log(2)*((t-41*200-delay)/tau1)**2)*np.cos(w2*(t-41*200-de

    #load band structure

    Ek=np.loadtxt('jicai_project/bandstructure5.txt')
```

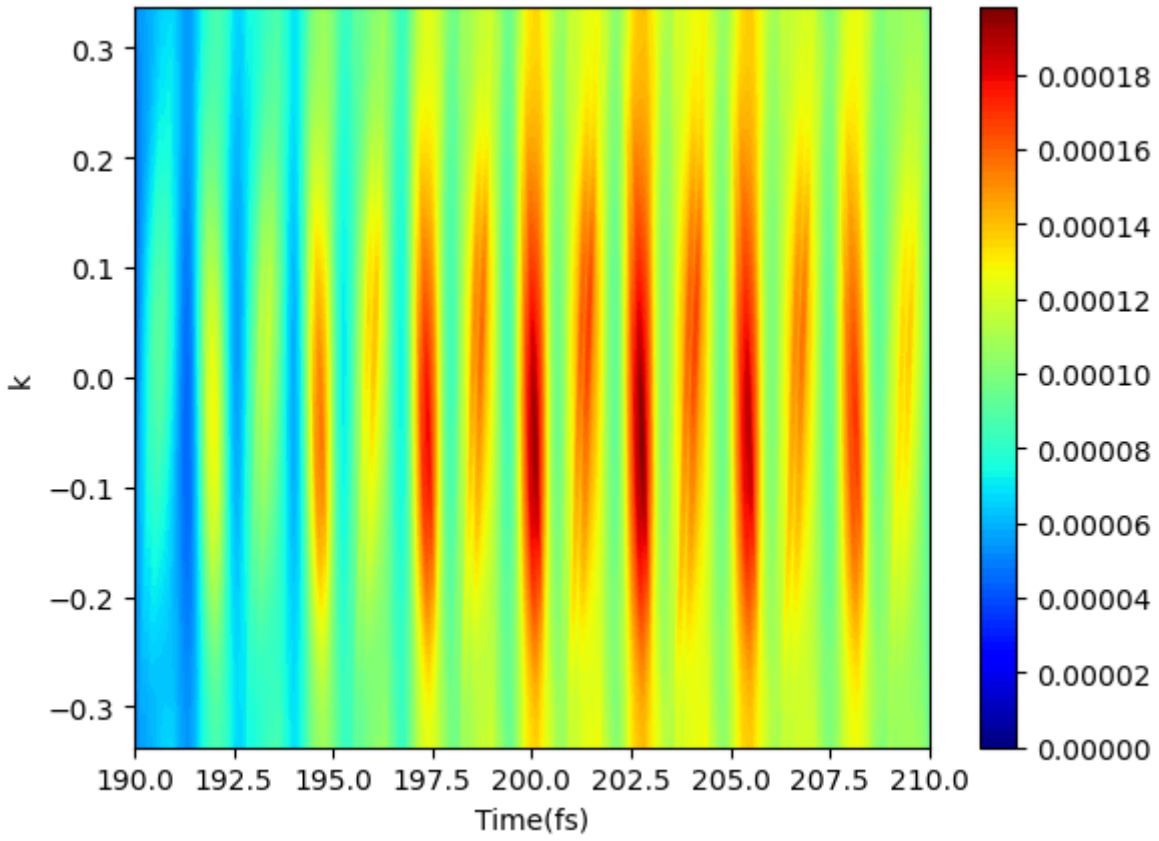
```
Ek=np.hstack((np.flip(Ek[:,1:],axis=1),Ek))/27.21 #symmetry band structure


VB=np.array(Ek[0:3])#assign VB
CB=np.array(Ek[3:])#assign CB









#set mapping matrix
MP=np.linspace(0,len(Ek)**2-1,len(Ek)**2,dtype=int).reshape((len(Ek),len(Ek)))

#set transition dipole matrix

dipole=np.array([np.zeros(k.size) for i in range(len(Ek)**2)])     #dipole shou

#K-p theory
for p in range(len(Ek)):
    for q in range(len(Ek)):
        if p==q:
            pass
        else:
            if p<=2 and q<=2: #use condition to set different value of dipole f
                dipole[MP[p,q]]=0.1*(Ek[p,100]-Ek[q,100])/(Ek[p]-Ek[q])
            else:
                dipole[MP[p,q]]=0.1*(Ek[p,100]-Ek[q,100])/(Ek[p]-Ek[q])









#set dephasing time
T2=41*2
#relaxation time
T1=41*5

#set coulomb potential(FFT of 1D soft Coulomb)
Vkq=np.ones((k.size,k.size))*(0+0j)
V0=0.1
for p in range(k.size):
    Vkq[p]=V0*dk/2/pi*2*scipy.special.kn(0,np.abs(k[p]-k))   #kn is modified Be
Vkq[np.diag_indices_from(Vkq)]=0+0j


#set filter for FFT when calculating Pw and Jw
gauss=np.exp(-4*np.log(2)*((t-41*200)/180/41)**12)

SBEg=SBE(d,VB,CB,dipole,k,E0field,E1field,T2,T1,t,Vkq)  #create a SBE object
SBEg.solve()                                              #solve the PDE
SBEg.calculate(gauss)                                     #calculate the P(t),
SBEg.showEfield(rangex=(1,2))                            #plot the electric fiel
SBEg.showEnergy()                                         #plot all the energy
SBEg.plotelectrondensity(n=0,rangex=(190,210))                #plot the electr
SBEg.plotemission(rangex=(0,15))                         #plot P(t),J(t),P(ω)
```


Electricfield
A.U.
0.02
0.01
0.00
−0.01
0
50
100
150
200
250
300
350
400
8
6
4
2
0
1.0
1.2
1.4
1.6
1.8
2.0
eV

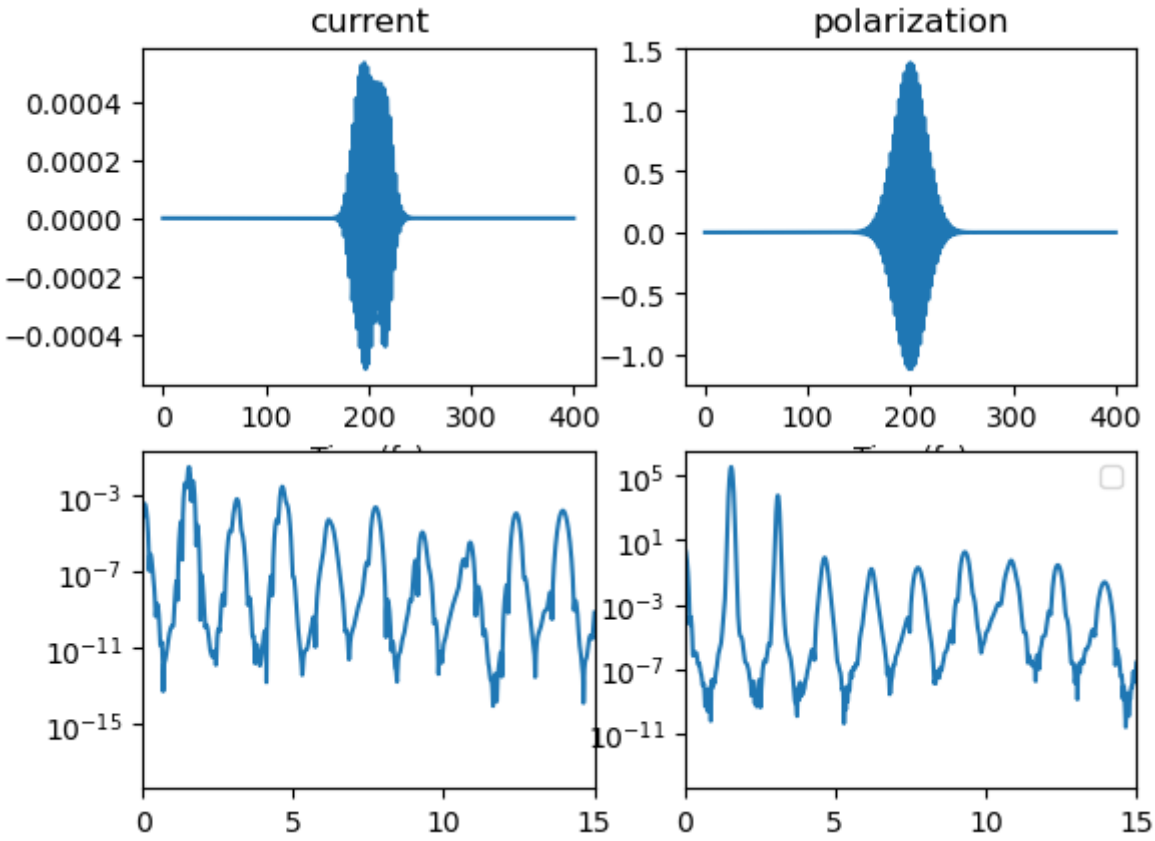

Bandstructure
energy(eV)
6
4
2
0
−2
−4
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
k(π/d)




```
C:\Users\Wenqi\anaconda3\lib\site-packages\numpy\ma\core.py:2829: ComplexWarning: Ca
sting complex values to real discards the imaginary part
  _data = np.array(data, dtype=dtype, copy=copy,
```




```
C:\Users\Wenqi\anaconda3\lib\site-packages\matplotlib\cbook\__init__.py:1298: Comple
xWarning: Casting complex values to real discards the imaginary part
  return np.asarray(x, float)
No artists with labels found to put in legend.  Note that artists whose label start
with an underscore are ignored when legend() is called with no argument.
```



Parameters Input

IMPORTANT NOTE: When you create a new array in numpy, it is a row vector.

Load Band Structure

In the **SBEwithCI** module, the **loadband** function is provided to help you load the bandstructure from txt file. The txt file should have 2 column, first column is the k points and second one is the value of energy. The

In [1]:
```
def loadband(k,filename):
    band=np.loadtxt(filename).T                          #load txt data
    band[1]=savgol_filter(band[1],11,1)                  #smooth data
    f=interpolate.interp1d(band[0],band[1])              #Interpolation for your s
    newband=f(k)
    return newband

CB1=loadband(k,'bandstructure\\CB1.txt')                  #It will load the CB1 fr
```

After you load all the energy band respectively, you should put them in Valence/Conduct band matrix. I recommend to put them in order of energy. Then create a matrix include all the energy bands.

In [ ]:
```
VB=np.array([VB1,VB2,VB3,.....])
CB=np.array([CB1,CB2,CB3,.....])
Ek=np.vstack((VB,CB))
```

Transition Dipole Matrix Element

The TDM should have n*n rows and k-points columns. And the rule for the sequence is shown in following table.

Suppose that the system only have 3 energy bands.

Row in TDM	Assignment
Row1	Dipole for 1st band to 1st band
Row2	Dipole for 1st band to 2nd band
Row3	Dipole for 1st band to 3rd band
Row4	Dipole for 2nd band to 1st band
Row5	Dipole for 2nd band to 2nd band
Row6	Dipole for 2nd band to 3rd band
Row7	Dipole for 3rd band to 1st band
Row8	Dipole for 3rd band to 2nd band
Row9	Dipole for 3rd band to 3rd band

You can also use the Mapping Matrix to set the dipole. `Mapping(0,1)` is exactly equal to 1, so that `dipole[Mapping(0,1)]` represent the Row2 of TDM, here the `0` and `1` represent the first and second band.

Coulomb Potential

Here we employ the Coulomb interaction as

$$V_{k,k'} = V_0 \frac{dk}{2\pi} 2K_0(|k - k'|)$$

where V_0 is the strength of the electron-hole interaction, and K_0 is the modified Bessel function of the second kind.

The coulomb matrix could be created by a simple loop.

In [ ]:
```
Vkq=np.ones((k.size,k.size))*(0+0j)
V0=1.8
for p in range(k.size):
    Vkq[p]=V0*dk/2/pi*2*scipy.special.kn(0,np.abs(k[p]-k))
Vkq[np.diag_indices_from(Vkq)]=0+0j
```

SBE class

SBEg=SBE(d,VB,CB,dipole,k,E0field,E1field,T2,T1,t,Vkq)

As shown in above the SBE object have 11 parameters. And their form is shown in the following Table.

Parameters	Form
lattice constant:d	constant

Parameters	Form
Valence Band:VB	N1 by k matrix
Conduct Band:CB	N2 by k matrix
Transition Dipole Moment:Dipole	(N1+N2)^2 by k matrix
k-points:k	1 by k matrix
Electic field 0:E0field	1 by t matrix
Electic field 1:E1field	1 by t matrix
Coherence Dephasing Time:T2	constant
Relaxation Time:T1	constant
time:t	1 by t matrix
Coulomb Potential:Vkq	k by k matrix

Properties

Besides the above parameters, the SBE class also have many properties which are shown in following table.

Variable name	Meaning
Vg	Group Velocity of all the energy bands
Efield	Totol electric field
freqs	fft of time
energy	freqs 2π 27.21 (eV)
Pt	Polarization
Pw	fft of Pt
SwP	|Pw|^2
Jt	Current
Jw	fft of Jt
SwJ	|Jw|^2
absorption	absorption spectrum

All the properties can be call by

`SBEg=SBE(d,VB,CB,dipole,k,E0field,E1field,T2,T1,t,Vkq)` \ `SBEg.xxxx (xxxx=properties' name)`

Solving the PDE

After create a new SBE object, one should use `SBEg.solve()` to solve the PDE.

In [1]:
```
    def solve(self):
        self.calculateddt()                              #calculate energy difference
        self.hindex=np.linspace(0, self.fhN-1,self.fhN,dtype=int)
        self.eindex=np.linspace(self.fhN, self.feN+self.fhN-1,self.feN,dtype=int)
```

```
        self.parameter1=(self.bandN,self.kN,self.T1,self.dk)
        self.parameter2=(self.time,self.Efield,self.dipole,self.ddt,self.MP,self.Vk
        self.sol=solve_ivp(finiteSBE, (self.time[0],self.time[-1]),self.y0, t_eval=
```

```
  File "C:\Users\Wenqi\AppData\Local\Temp\ipykernel_38564\225012329.py",
line 7
    self.sol=solve_ivp(finiteSBE, (self.time[0],self.time[-1]),self.y0, t
_eval=self.time,atol=1e-10,rtol=1e-12,args=(self.parameter1,self.paramete
r2) #use solve_ivp to solve the PDE, change the atol and rtol to control
the accuracy

^
SyntaxError: unexpected EOF while parsing
```

The details of the SBE PDE is in `finiteSBE.py`, and it use the `numba.njit` to compile the derivative equations function to machine code.

Calculating the result

After solve the PDE, you should use `SBEg.calculate(filter)` to calculate the P(t),J(t),d(t),P(ω), J(ω),d(ω), and absorption spectrum.

In [ ]:
```
    def calculate(self,Filter):
        y=self.sol.y.T
        self.Pt=np.zeros(self.sol.t.size,dtype=complex)
        self.Jt=np.zeros(self.sol.t.size,dtype=complex)
        self.fkt=np.zeros((self.sol.t.size,self.bandN*self.kN),dtype=complex)
        self.pkt=np.zeros((self.sol.t.size,self.bandN**2*self.kN),dtype=complex)
        for i in range(len(self.sol.t)):
            yi=np.reshape(y[i],(self.bandN**2+self.bandN,self.kN))
            pk=yi[0:self.bandN**2]
            fk=yi[self.bandN**2:]
            self.Pt[i]=np.real(np.sum(np.sum(self.dipole*pk,1)))
            #self.Pt[i]=np.sum(np.sum(self.dipole*pk,1))
            self.Jt[i]=np.real(np.sum(np.sum(self.Vg*fk,1)))
            #self.Jt[i]=np.sum(np.sum(self.Vg*fk,1))
            self.pkt[i]=pk.reshape(pk.size)
            self.fkt[i]=fk.reshape(fk.size)
        self.Pw=fftshift((fft(self.Pt*Filter)))
        self.Jw=fftshift((fft(self.Jt*Filter)))
        self.SwP=np.abs(self.Pw)**2
        self.SwJ=np.abs(self.Jw)**2
        self.dt=difft(self.Pt,self.time)+self.Jt
        self.dw=fftshift((fft(self.dt*Filter)))
        self.Sw=np.abs(self.dw)**2
        self.Ew=fftshift(fft(self.E0))
        self.absorption=self.freqs*np.imag(self.Pw/self.Ew)
```

Plot the result

The SBE class provide several method to help you plot your result.

In [ ]:
```
    def showEfield(self,rangex): #plot the electric field
        plt.figure(1)
        plt.subplot(2,1,1)
        plt.plot(self.time/41,self.Efield)
        plt.title('Electricfield')
        plt.ylabel('A.U.')
        plt.xlabel('Time(fs)')
```

```
        plt.subplot(2,1,2)
        plt.plot(self.freqs*2*pi*27.21,np.abs(fftshift(fft(self.Efield))))
        plt.xlabel('eV')
        plt.xlim(rangex[0],rangex[1])
        plt.show()
```

In [ ]:
```
    def showEnergy(self): #plot the bandstructure
        plt.figure()
        Matplot(self.Ek*27.21,self.k/pi*self.d)
        plt.title('Bandstructure')
        plt.xlabel('k(π/d)')
        plt.ylabel('energy(eV)')
        plt.figure()
        Matplot(self.Vg,self.k/pi*self.d)
        plt.title('Group Velocity')
        plt.ylabel('A.U.')
        plt.xlabel('k(π/d)')
        plt.show()
```

In [ ]:
```
    def plotelectrondensity(self,n,rangex):  #plot electronsity on n-th band with ti
        plt.figure(2)
        self.fkn=(self.fkt.T)[n*self.kN:(n+1)*self.kN]
        T,K=np.meshgrid(self.time,self.k)
        plt.contourf(T/41,K,self.fkn,cmap=cm.jet,levels=2**7);
        plt.ylabel('k')
        plt.xlabel('Time(fs)')
        plt.xlim(rangex[0],rangex[1])
        plt.colorbar()
        plt.show()
```

In [ ]:
```
    def plotcoherence(self,n,rangex):
        plt.figure(3)
        self.pkn=(self.pkt.T)[n*self.kN:(n+1)*self.kN]
        T,K=np.meshgrid(self.time,self.k)
        plt.contourf(T/41,K,self.pkn,cmap=cm.jet,levels=2**7);
        plt.ylabel('k')
        plt.xlabel('Time(fs)')
        plt.xlim(rangex[0],rangex[1])
        plt.colorbar()
        plt.show()
```

In [ ]:
```
    def plotemission(self,rangex):#plot Pt,Jt,SwP,SwJ
        plt.figure(3)
        plt.subplot(2,2,1)
        plt.plot(self.sol.t/41,self.Jt)
        plt.title("current")
        plt.xlabel("Time(fs)")
        plt.subplot(2,2,2)
        plt.plot(self.sol.t/41,self.Pt)
        plt.title("polarization")
        plt.xlabel("Time(fs)")
        plt.subplot(2,2,3)
        plt.semilogy(self.energy,self.SwJ)
        plt.xlim(rangex[0],rangex[1])
        plt.subplot(2,2,4)
        plt.semilogy(self.energy,self.SwP)
        plt.xlim(rangex[0],rangex[1])
        plt.legend()
        plt.show()
```

In [ ]:
```
    def plotabsorption(self,rangex,rangey):#plot absorption of probe with x-range ar
        plt.figure(4)
```

```
        plt.plot(self.freqs*2*pi*27.21,self.absorption)
        plt.xlim(rangex[0],rangex[1])
        plt.ylim(rangey[0],rangey[1])
        plt.show()
```

Parameters Scan

Here I provide a example for parameter scan.

In [ ]:

```
# -*- coding: utf-8 -*-
"""
Created on Mon Sep 18 12:40:42 2023

@author: Wenqi
"""



import numpy as np
import scipy
from matplotlib import pyplot as plt
from math import sqrt
from SBEwithCI import SBE, loadband, Matplot
import time as tp
import copy
from multiprocessing import Pool
import multiprocessing as mp
from matplotlib import cm

from numpy.fft import fft, fftfreq,fftshift,ifft


#A simple SBE simulation should be done before start the scan
def pumpprobe(SBEg,delay,pumpI,probeI,V0,T2,T1): #funcition of scan the parameter (d


    t=SBEg.time
    gauss=np.exp(-4*np.log(2)*((t-41*200)/180/41)**12)
    w1=0.057       #frequency
    tau=41*25*sqrt(2) #pulse duration
    fi=0               #phase
    E0=1e9*pumpI             #field strength, pumpI is the intensity factor
    E0field=np.exp(-4*np.log(2)*((t-41*200)/tau)**2)*np.cos(w1*(t-41*200)+fi)/5.14

    #set electric field 1 (optional)
    w2=0.057*2         #frequency
    tau1=41*30*sqrt(2) #pulse duration
    fi1=0             #phase
    E1=1e9*probeI    #field strength, probeI is the intensity factor
    E1field=np.exp(-4*np.log(2)*((t-41*200-delay)/tau1)**2)*np.cos(w2*(t-41*200-de

    SBE1=copy.deepcopy(SBEg)

    SBE1.T2=T2
    SBE1.T1=T1
    SBE1.Vkq=V0*SBE1.Vkq #Coulomb matrix, V0 is the strength factor
    SBE1.E0=E0field
    SBE1.Efield=E0field+E1field#new Efield
    SBE1.solve()#solve PDEs
    SBE1.calculate(gauss)#calculate the P(t),J(t),d(t),P(ω), J(ω),d(ω), and absor
    return SBE1.SwP     #also can return like (SBE1.SwP,SBE1.SwJ,SBE1.Sw)
```

```
if __name__ == '__main__': #similar to main function in C/C++, multiprocessing need


    pi=scipy.constants.pi #pi constant
    d=9.32                  #lattice constant
    t=np.linspace(0,41*400,10000) #time axis
    k=np.linspace(-pi/d, pi/d,201)    #k axis
    dk=k[1]-k[0]


    #set electric field 0
    w1=0.057       #frequency
    tau=41*25*sqrt(2) #pulse duration
    fi=0               #phase
    E0=1e10             #field strength
    E0field=np.exp(-4*np.log(2)*((t-41*200)/tau)**2)*np.cos(w1*(t-41*200)+fi)/5.14

    #set electric field 1 (optional)
    w2=0.057*2         #frequency
    tau1=41*30*sqrt(2) #pulse duration
    fi1=0              #phase
    E1=1e9          #field strength
    delay=0          #delay between two pulses
    E1field=np.exp(-4*np.log(2)*((t-41*200-delay)/tau1)**2)*np.cos(w2*(t-41*200-de

    #load band structure

    Ek=np.loadtxt('jicai_project/bandstructure5.txt')
    Ek=np.hstack((np.flip(Ek[:,1:],axis=1),Ek))/27.21 #symmetry band structure


    VB=np.array(Ek[0:3])#assign VB
    CB=np.array(Ek[3:])#assign CB




    #set mapping matrix
    MP=np.linspace(0,len(Ek)**2-1,len(Ek)**2,dtype=int).reshape((len(Ek),len(Ek)))

    #set transition dipole matrix

    dipole=np.array([np.zeros(k.size) for i in range(len(Ek)**2)])     #dipole shou

    #K-p theory
    for p in range(len(Ek)):
        for q in range(len(Ek)):
            if p==q:
                pass
            else:
                if p<=2 and q<=2: #use condition to set different value of dipole f
                    dipole[MP[p,q]]=0.1*(Ek[p,100]-Ek[q,100])/(Ek[p]-Ek[q])
                else:
                    dipole[MP[p,q]]=0.1*(Ek[p,100]-Ek[q,100])/(Ek[p]-Ek[q])
```

```
#set dephasing time
T2=41*2
#relaxation time
T1=41*5

#set coulomb potential(FFT of 1D soft Coulomb)
Vkq=np.ones((k.size,k.size))*(0+0j)
V0=0.1
for p in range(k.size):
    Vkq[p]=V0*dk/2/pi*2*scipy.special.kn(0,np.abs(k[p]-k))   #kn is modified Be
Vkq[np.diag_indices_from(Vkq)]=0+0j


#set filter for FFT when calculating Pw and Jw
gauss=np.exp(-4*np.log(2)*((t-41*200)/180/41)**12)

SBEg=SBE(d,VB,CB,dipole,k,E0field,E1field,T2,T1,t,Vkq)  #create a SBE object
SBEg.solve()                                              #solve the PDE
SBEg.calculate(gauss)                                     #calculate the P(t),
SBEg.showEfield(rangex=(1,2))                            #plot the electric fiel
SBEg.showEnergy()                                         #plot all the energy
SBEg.plotelectrondensity(n=0,rangex=(190,210))                 #plot the electr
SBEg.plotemission(rangex=(0,15))                         #plot P(t),J(t),P(ω)


delaytime=np.linspace(-80,80,41)*41 #set delay time points
V0=[0,7]                          #set Coulomb strength scan
pumpI=[1,2,3,4,5,6,7,8,9,10]  #set pump intensity factor scan
probeI=[3,4,5,6,7,8]         #set probe intensity factor scan
T2scan=np.array([2])*41      #set T2 scan
T1scan=np.array([2,5])*41    #set T1 scan

scan=[(SBEg,tpoints,pumpIpoints,probeIpoints,V0points,T2points,T1points) for T1p
for i in range(len(V0)*len(pumpI)*len(probeI)*len(T2scan)*len(T1scan)): #do del
    pool=Pool(4) #4 processing
    scanparameter=scan[41*i:41*(i+1)]
    Vpoints=scanparameter[0][4]
    pumpIpoints=scanparameter[0][2]
    probeIpoints=scanparameter[0][3]
    T2points=scanparameter[0][5]
    T1points=scanparameter[0][6]
    pp=pool.starmap(pumpprobe, scanparameter) #multiprocessing calculation, resu

    pool.close() # pool close
    pool.join() #pool close
    #save the delay scan
    np.save('jicai_project//5bands//scan3//pumpI='+str(pumpIpoints)+'e9'+'probeI
```