HW-1

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Problem 11

Consider a potential (take $L = 8nm$)

$$U(x) = \begin{cases} U_0 = 400meV & x < 0 \& x > L \\ 0 & 0 < x < L \end{cases}$$

a)By solving Schrödinger's equation, find the lowest eigenvalue (energy level) and the corresponding eigenfunction.

b)Plot the eigenfunction using a plotting package. Ensure that you present a zoomed-in plot of the eigenfunction for $x < 0$ and $x > L$.

c) Show that the eigenvalues form a discrete spectrum for energies less than U_0 and a continuous spectrum for higher energies. That is, for this Hamiltonian, there are both discrete quantum numbers with eigenenergies smaller than U_0 and a continuum of quantum numbers with eigenenergies larger than U_0.

Solution

A) Xichen Li: I am the only person in my group. I wrote the problem by myself. I started the problem by solving the eigenvalue and eigenfunction of the time-independent Schrödinger equation and then process the solved results.

a) Solve timd-indepednent Schrödinger equation:

For $0 < x < L$

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}]\psi(x) = E\psi(x)$$
$$-\frac{\partial^2}{\partial x^2}\psi(x) = k_1^2\psi(x)$$

Where $k_1 = \frac{2mE}{\hbar^2}$, and then the general solution for $\psi(x)$ can be written as :

$$\psi(x) = A_1 sin(k_1 x) + B_1 cos(k_1 x)$$

For $x < 0$ and $x > L$

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0]\psi(x) = E\psi(x)$$
$$-\frac{\partial^2}{\partial x^2}\psi(x) = k_2^2\psi(x)$$

Where $k_2 = \frac{2m(E-U_0)}{\hbar^2}$, and then the general solution for $\psi(x)$ can be written as :

$$\psi(x) = A_2 sin(k_2 x) + B_2 cos(k_2 x)$$

Boundary Condition 1: $\psi(0^+) = \psi(0^-)$

$$A_1 sin(0) + B_1 cos(0) = A_2 sin(0) + B_2 cos(0)$$

Then $B_1 = B_2$. Boundary Condition 2: $\psi(L^+) = \psi(L^-)$

$$A_1 sin(k_1 L) + B_1 cos(k_1 L) = A_2 sin(k_2 L) + B_2 cos(k_2 L)$$

It seems hard to determine all the parameters from the two boundary conditions, so the above time-independent Schrödinger equation is solved numerically which is shown below:

In [33]:
```
import numpy as np
%matplotlib notebook
import matplotlib.pyplot as plt
```

In [34]:
```
N = 200  # Grid size is 100
L = 8e-9

def V(x): # Return the potential energy given the position of each grid element
    if x<0 or x >L :
      result = 400e-3 * 1.6e-19
    else:
      result = 0
    return result

eta = 6.63e-34/2/np.pi #Reduced Plank constant in eV.s
m = 9.11e-31   #Assuming the particle mass is equal to a free electron
q = 1.6e-19
```

In [35]:
```
X = np.linspace(-2*L,2*L,num=N)
a = X[1] - X[0] # grid spacing

#print(X)

U=[]
U=np.array(U, dtype=float)

for x in X:
    U=np.append(U,V(x))

#print(U)

t = -eta**2 / (2 * m * a**2)
eps = -2*t + U

#print(t)
```

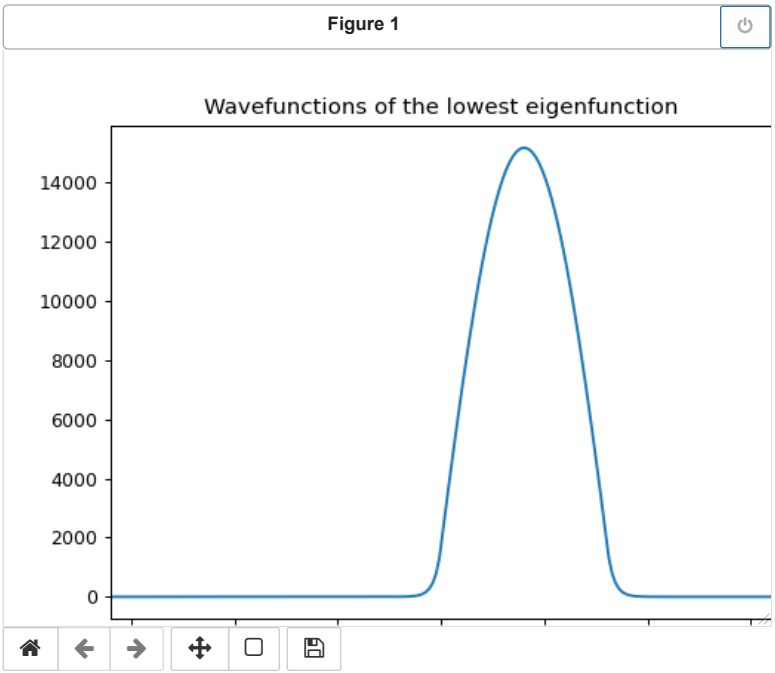
In [36]:
```
H = t*np.eye(N, k=-1) + eps*np.eye(N) + t*np.eye(N, k=1) # discretized hamiltonian
#plt.matshow(H)
```

In [37]:
```
vals, vecs = np.linalg.eig(H) # Solve for Eigen function and eigen values
#print(vals)
#print(vals.shape)
#print(vecs)
#print(vecs.shape)
order = np.argsort(vals)
vals, vecs = vals[order], vecs[:, order] # sort the eigen value and eigen functions
#print(vals)
#print(vecs)
vecs = vecs.T # Transpose
vecs /= np.sqrt(a) #Normalize
vals_eV=vals/1.6e-19
#print (vals_eV)
#print(vecs[0])
p = np.abs(vecs)**2
probs = a*p
#print(sum(probs[0]))
```

Now we have the eigenvalues (which correspond to the energies of each state) and the eigenvectors (which are the states, aka wavefunctions).

In [38]:
```
print ("The lowest energy is {:.4f}eV".format(vals_eV[0]))
print ("The corresponding eigenfunction is {}".format(vecs[0]))
print ("Verfiy the summed probablity of the frist eigenfunction: {} is equal to 1".format(sum(probs[0])))
#plot the first eigenfunction magnitude
plt.figure()
plt.plot(X,vecs[0],'-')
plt.title('Wavefunctions of the lowest eigenfunction')
plt.xlabel('x')
plt.xlim([-2*L,2*L])
#plt.ylim([-7000,-4000])
```

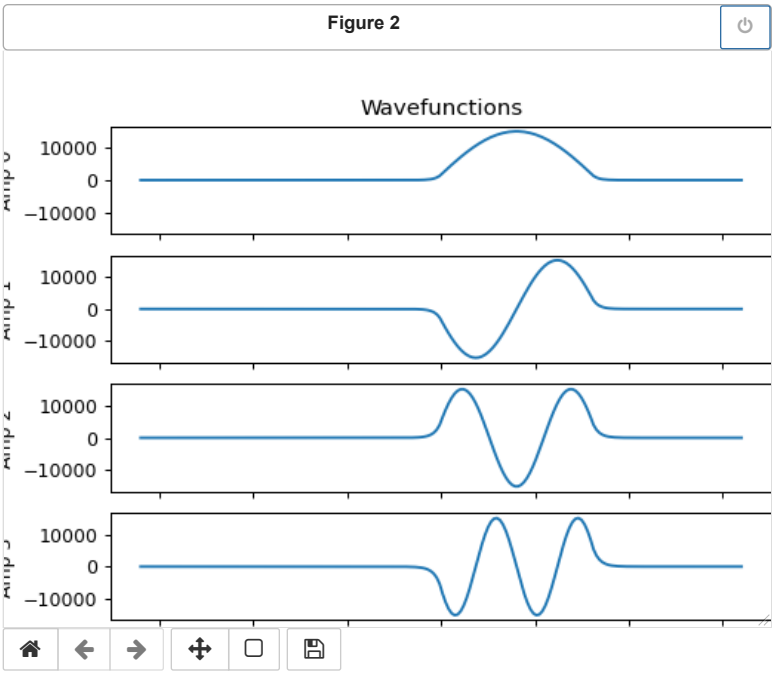
```
The lowest energy is 0.0050eV
The corresponding eigenfunction is [-8.85592456e-11 -9.56054439e-11 -2.73299246e-11 -8.85605770e-11
 -5.67051899e-11  8.70094459e-12 -2.89183510e-11  1.38468949e-11
  1.84631629e-11  4.99044984e-11  9.52652336e-11  2.33326032e-11
  4.26402148e-11  2.35197976e-11 -6.28774556e-11 -2.66508167e-11
 -3.11814721e-11 -4.69053865e-11 -2.73870223e-11 -2.01532618e-11
  2.00232354e-11 -3.65512120e-11 -7.35270988e-11 -6.10492213e-11
 -4.37056890e-11 -1.90932311e-11 -7.23852865e-11 -2.71908295e-11
  1.82036282e-11 -3.56714229e-11 -1.78354207e-11 -1.64046124e-11
  6.75728594e-12  4.77352903e-11 -2.14985904e-12 -2.36968056e-11
  3.55318728e-11  5.11381690e-11  2.52075869e-11  1.39434084e-13
  3.26102925e-11  1.22714183e-10  2.01387216e-10  3.90319428e-10
  7.71641285e-10  1.29694819e-09  2.16912663e-09  3.64142754e-09
  6.10430121e-09  1.02215345e-08  1.70713663e-08  2.85435421e-08
  4.75884047e-08  7.93380505e-08  1.32307232e-07  2.20590708e-07
  3.67980098e-07  6.13780429e-07  1.02363946e-06  1.70737357e-06
  2.84759421e-06  4.74929185e-06  7.92106771e-06  1.32110136e-05
  2.20339120e-05  3.67489628e-05  6.12912983e-05  1.02224099e-04
  1.70493265e-04  2.84355354e-04  4.74259052e-04  7.90987792e-04
  1.31924053e-03  2.20028115e-03  3.66971518e-03  6.12049495e-03
  1.02080016e-02  1.70253056e-02  2.83954726e-02  4.73590832e-02
  7.89873369e-02  1.31738179e-01  2.19718104e-01  3.66454474e-01
  6.11187148e-01  1.01936190e+00  1.70013178e+00  2.83554648e+00
  4.72923566e+00  7.88760477e+00  1.31552567e+01  2.19408532e+01
  3.65938158e+01  6.10326016e+01  1.01792567e+02  1.69773637e+02
  2.83155133e+02  4.72257240e+02  7.87649153e+02  1.31367216e+03
  2.19099396e+03  3.06089609e+03  3.92043268e+03  4.76669295e+03
  5.59681108e+03  6.40797594e+03  7.19744056e+03  7.96253147e+03
  8.70065773e+03  9.40931971e+03  1.00861176e+04  1.07287594e+04
  1.13350689e+04  1.19029928e+04  1.24306080e+04  1.29161276e+04
  1.33579075e+04  1.37544516e+04  1.41044170e+04  1.44066187e+04
  1.46600332e+04  1.48638024e+04  1.50172361e+04  1.51198148e+04
  1.51711912e+04  1.51711912e+04  1.51198148e+04  1.50172361e+04
  1.48638024e+04  1.46600332e+04  1.44066187e+04  1.41044170e+04
  1.37544516e+04  1.33579075e+04  1.29161276e+04  1.24306080e+04
  1.19029928e+04  1.13350689e+04  1.07287594e+04  1.00861176e+04
  9.40931971e+03  8.70065773e+03  7.96253147e+03  7.19744056e+03
  6.40797594e+03  5.59681108e+03  4.76669295e+03  3.92043268e+03
  3.06089609e+03  2.19099396e+03  1.31367216e+03  7.87649153e+02
  4.72257240e+02  2.83155133e+02  1.69773637e+02  1.01792567e+02
  6.10326016e+01  3.65938158e+01  2.19408532e+01  1.31552567e+01
  7.88760477e+00  4.72923566e+00  2.83554648e+00  1.70013178e+00
  1.01936190e+00  6.11187148e-01  3.66454474e-01  2.19718104e-01
  1.31738179e-01  7.89873370e-02  4.73590831e-02  2.83954726e-02
  1.70253056e-02  1.02080016e-02  6.12049495e-03  3.66971520e-03
  2.20028112e-03  1.31924053e-03  7.90987859e-04  4.74258992e-04
  2.84355412e-04  1.70493255e-04  1.02224032e-04  6.12913102e-05
  3.67489334e-05  2.20338547e-05  1.32109981e-05  7.92102494e-06
  4.74928849e-06  2.84749834e-06  1.70727129e-06  1.02360776e-06
  6.13599403e-07  3.67717264e-07  2.20196710e-07  1.31492745e-07
  7.80180023e-08  4.53123036e-08  2.48597063e-08  1.09424476e-08]
Verfiy the summed probablity of the frist eigenfunction: 1.0000000000000002 is equal to 1
```



Out[38]: (-1.6e-08, 1.6e-08)

b) Plot the eigenfunction of the lowest four eigenfunctions.

In [39]:
```
fig, axes = plt.subplots(4, sharex=True, sharey=True)
plt.sca(axes[0])
plt.title('Wavefunctions')
for i, (ax, Amp, E) in enumerate(zip(axes, vecs, vals_eV)):
    plt.sca(ax)
    plt.ylabel('Amp {}'.format(i))
    plt.plot(X, Amp)
    #plt.fill_between(X, psi, alpha=0.3)
    print('E_{} = {:.4f}'.format(i, E))
plt.xlabel('x')
```

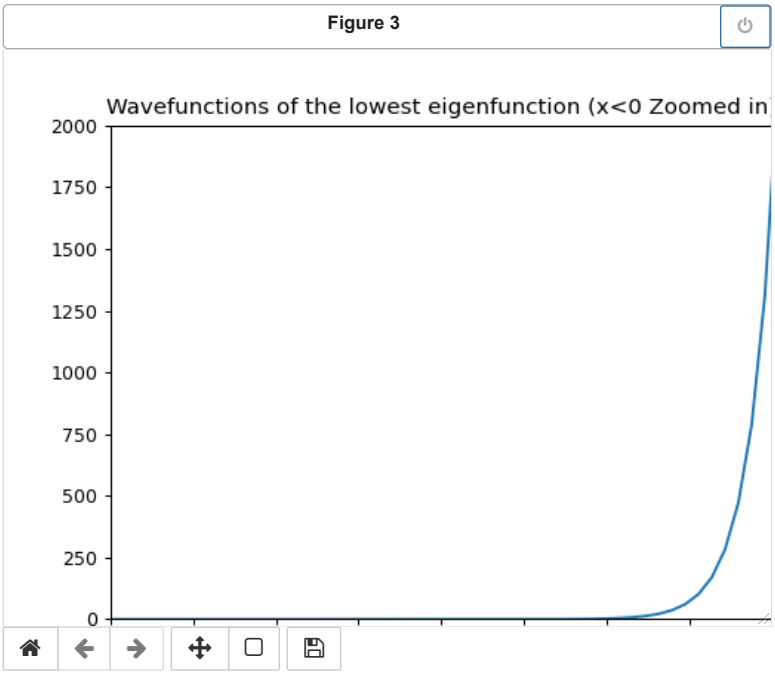



```
E_0 = 0.0050
E_1 = 0.0200
E_2 = 0.0448
E_3 = 0.0794
```

Out[39]: Text(0.5, 0, 'x')

A zoomed-in plot of the lowest eigenfunction for $x < 0$ is shown below:

In [40]:
```
plt.figure()
plt.plot(X,vecs[0],'-')
plt.title('Wavefunctions of the lowest eigenfunction (x<0 Zoomed in)')
plt.xlabel('x')
plt.xlim([-L,0])
plt.ylim([0,2000])
```

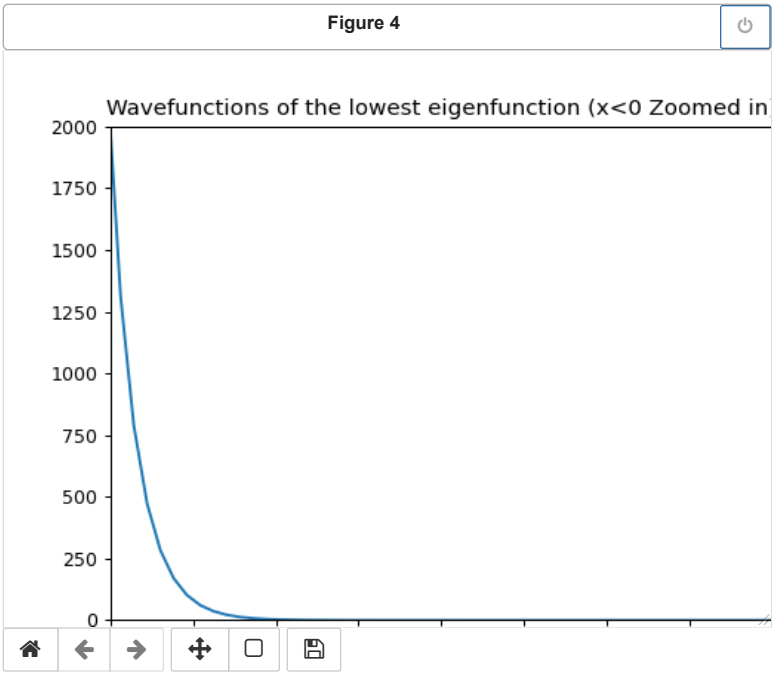


Out[40]: (0.0, 2000.0)

As you can see from the plotted figure above, the wavefunction is approaching zero at the boundary ($x = -L$).

A zoomed-in plot of the lowest eigenfunction for $x > L$ is shown below:

In [41]:
```
plt.figure()
plt.plot(X,vecs[0],'-')
plt.title('Wavefunctions of the lowest eigenfunction (x<0 Zoomed in)')
plt.xlabel('x')
plt.xlim([L,2*L])
plt.ylim([0,2000])
```



Out[41]: (0.0, 2000.0)

As you can see from the plotted figure above, the wavefunction is approaching zero at the boundary ($x = 2L$).

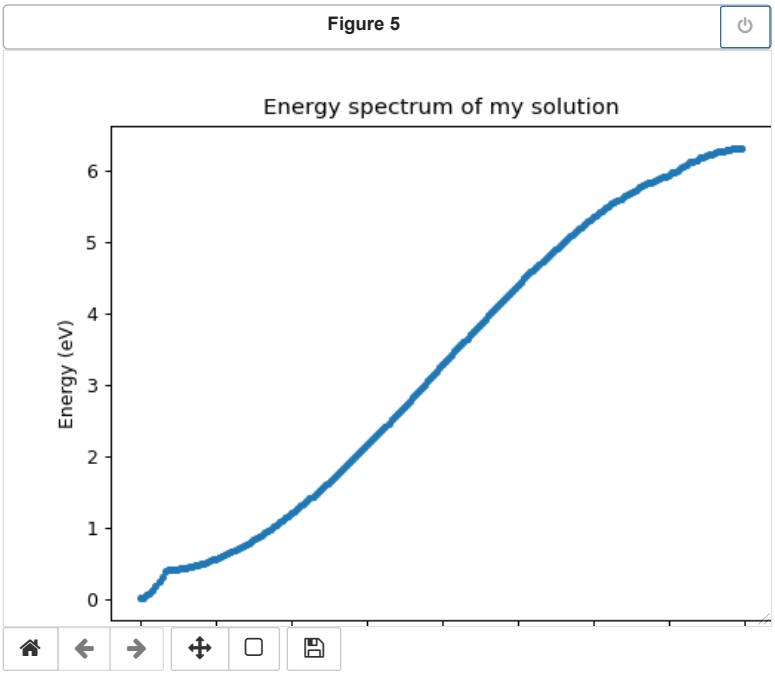
c)Show the eigenvalues form a discrete spectrum for energies less than U_0 and a continuous spectrum for higher energies

In [42]:
```
#cutoff = 20 # how many energy levels to trust from our computed results (probably shouldn't be more than 20 or so)
#psi = vecs[:cutoff].astype(np.complex64)
#E_eV = vals_eV[:cutoff]
print ("The eigenvalues are {}eV for N={}".format(vals_eV,N))
```

```
The eigenvalues are [5.00205895e-03 1.99759907e-02 4.48227110e-02 7.93681557e-02
 1.23345067e-01 1.76352553e-01 2.37754732e-01 3.06352920e-01
 3.78419534e-01 4.01461685e-01 4.05510961e-01 4.06114925e-01
 4.12954704e-01 4.21414847e-01 4.23727532e-01 4.34883446e-01
 4.44782678e-01 4.51940421e-01 4.62833190e-01 4.73918583e-01
 4.89548207e-01 4.97441908e-01 5.15552832e-01 5.32801844e-01
 5.44446292e-01 5.62639144e-01 5.79099416e-01 6.00223479e-01
 6.13535463e-01 6.37341665e-01 6.57977024e-01 6.77557173e-01
 6.97627588e-01 7.21404188e-01 7.47087260e-01 7.66254635e-01
 7.93066866e-01 8.17157418e-01 8.45295939e-01 8.66629270e-01
 8.97320489e-01 9.23995949e-01 9.52820725e-01 9.77998159e-01
 1.01036234e+00 1.04046765e+00 1.06965209e+00 1.09916652e+00
 1.13235797e+00 1.16562038e+00 1.19552234e+00 1.22903750e+00
 1.26305848e+00 1.29887786e+00 1.32996538e+00 1.36680606e+00
 1.40194187e+00 1.43975344e+00 1.47238781e+00 1.51186218e+00
 1.54836815e+00 1.58774470e+00 1.62212907e+00 1.66366189e+00
 1.70166419e+00 1.74230907e+00 1.77850084e+00 1.82165438e+00
 1.86115477e+00 1.90286278e+00 1.94080658e+00 1.98525630e+00
 2.02616664e+00 2.06878606e+00 2.10834806e+00 2.15384886e+00
 2.19602415e+00 2.23942951e+00 2.28042536e+00 2.32678271e+00
 2.37004485e+00 2.41412011e+00 2.45633502e+00 2.50338419e+00
 2.54753692e+00 2.59216639e+00 2.63536829e+00 2.68296103e+00
 2.72779868e+00 2.77286283e+00 2.81681042e+00 2.86480710e+00
 2.91011929e+00 2.95549362e+00 2.99994083e+00 3.04820636e+00
 3.09378041e+00 3.13933598e+00 3.18403421e+00 3.23243624e+00
 3.27805831e+00 3.32366313e+00 3.36836223e+00 3.41677055e+00
 3.46222633e+00 3.50774699e+00 3.55219575e+00 3.60048206e+00
 3.64555756e+00 3.69086057e+00 3.73480749e+00 3.78284460e+00
 3.82732769e+00 3.87228004e+00 3.91547525e+00 3.96313449e+00
 4.00681814e+00 4.05128624e+00 4.09348577e+00 4.14063107e+00
 4.18331964e+00 4.22716533e+00 4.26813963e+00 4.31461559e+00
 4.35613643e+00 4.39920841e+00 4.43875755e+00 4.48436773e+00
 4.52459162e+00 4.56670961e+00 4.60468812e+00 4.64915893e+00
 4.68803397e+00 4.72896308e+00 4.76531610e+00 4.80824269e+00
 4.84584566e+00 4.88526041e+00 4.92006670e+00 4.96084729e+00
 4.99744667e+00 5.03489264e+00 5.06839347e+00 5.10619088e+00
 5.14227853e+00 5.17716345e+00 5.20972347e+00 5.24356924e+00
 5.27971678e+00 5.31142110e+00 5.34332160e+00 5.37259122e+00
 5.40879613e+00 5.43715050e+00 5.46809357e+00 5.49351675e+00
 5.52763286e+00 5.55430207e+00 5.58270720e+00 5.60688905e+00
 5.63374295e+00 5.66313828e+00 5.68610278e+00 5.71059042e+00
 5.72933001e+00 5.75801509e+00 5.77895654e+00 5.79987251e+00
 5.81901782e+00 5.83288494e+00 5.85557794e+00 5.87497486e+00
 5.88552666e+00 5.89977038e+00 5.90589381e+00 5.92146102e+00
 5.96324812e+00 5.98122683e+00 6.00362239e+00 6.04189303e+00
 6.05526839e+00 6.07785289e+00 6.11139078e+00 6.12103860e+00
 6.14243197e+00 6.17092010e+00 6.17754026e+00 6.19680996e+00
 6.22006409e+00 6.22426739e+00 6.24065096e+00 6.25854392e+00
 6.26089584e+00 6.27372060e+00 6.28616250e+00 6.28720430e+00
 6.29585472e+00 6.30278583e+00 6.30304580e+00 6.30694772e+00]eV for N=200
```

By looking at the eigen-value for $N = 200$ cases, we can find for eigenvalue is smaller than $U_0 = 0.4eV$, the eigenvalues have discrete values which are $E_0 = 0.005eV$, $E_1 = 0.02eV$, $E_2 = 0.045eV$, $E_3 = 0.08eV$, $E_4 = 0.123eV$, $E_5 = 0.176eV$, $E_6 = 0.238eV$, $E_7 = 0.306eV$, and $E_7 = 0.378eV$. When eigenvalue is larger than $U_0 = 0.4eV$, the eigenvalues have continuous energy spectrum. The energy spectrum for $N = 200$ can alsobe found in the figure below, where we can see a discontinuity at $E = 0.4eV$ on the energy spectrum.

In [43]:
```
plt.figure()
plt.plot(vals_eV,'.')
plt.title('Energy spectrum of my solution')
plt.xlabel('Level')
plt.ylabel('Energy (eV)')
```



Out[43]: Text(0, 0.5, 'Energy (eV)')

In [ ]:

In [ ]: