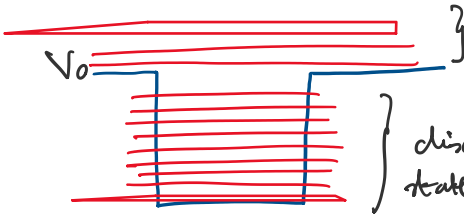
Script Python

Thursday 18 October 2018 22:56

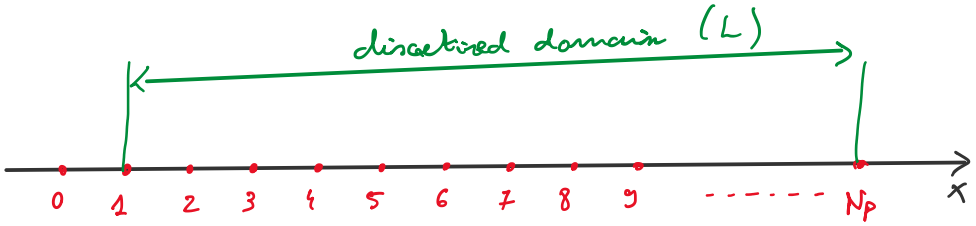
```
from numpy import *
from pylab import *

#I define the parameters
Np=300 #Number of grid points
L=20 #length of the discretized domain
W=10  #width of the potential well
hbar=1.05459e-34 #J/s
q=1.60219e-19    #C
m0=9.1095e-31    #Kg

#I create the grid
x=linspace(0,L,Np) # in nanometers

#I create the potential U(x) for the well
ind=nonzero(abs(x-L*0.5)>W*0.5);
U=zeros(Np);
U[ind]=10 #The height of the barrier is 10 eV


# Uncomment these three lines to plot the potential and exit
plot(x,U,'o-')
#show()
#exit(0);

#I create the hopping parameter -hbar**2/(2m0*a**2)
a=x[1]-x[0]
t=-hbar**2/(2*m0*(a*1e-9)**2)/q #eV

#I create the diagonal, updiagonal and lowdiagonal vectors
diago=(U-2*t)*(ones(Np));
lowdiag=t*ones(Np-1);
updiag=t*ones(Np-1);

#I create the Hamiltonian
H=diag(diago)+diag(lowdiag,-1)+diag(updiag,1)
H=array(H)
#H=mat(H)
[E,V]=eig(H)
print (hbar*pi/W*1e9)**2/2/m0/q min(E)
```

If you run the simulation you get something like this:



you get discrete states for energy $> V_0$, where you would have expected continuous states.
or in other words, you are getting discrete states, even though you have confinement.

What is going on?



for a point $1 < i < N_p$
the Schroedinger equation (discretized)

$$t\psi_{i-1} + (V - 2t)\psi_i + t\psi_{i+1} = E\psi_i$$

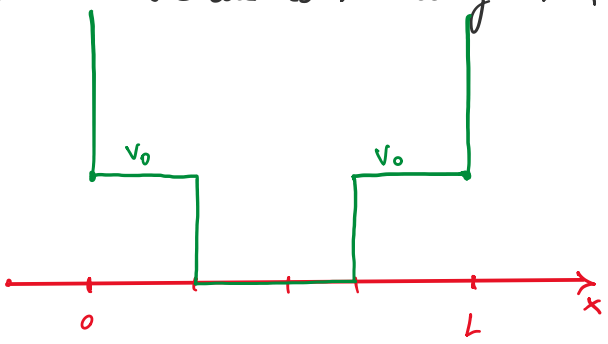
If $i = 1$: $(V - 2t)\psi_i + t\psi_{i+1} = E\psi_i$

or in other words $\boxed{\psi_0 = 0}$

And in the same way $\boxed{\psi_{N_p+1} = 0}$

$V_0 \to +\infty$ $\wedge$ $V_{N_p+1} \to +\infty$, i.e., Hard wall assumption

The real potential we are considering is the following:

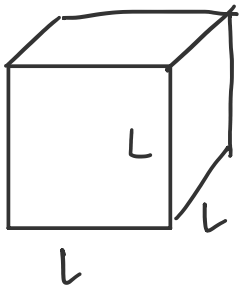


Homework: Compute the eigenvalues and eigenvectors of a harmonic potential and compare results with analytical solution.
What is the difference (if any)?

USEFULL RULE

Wednesday, 24 October 2018 15:19

$$I = \sum_k f(k)$$



$$k_x = \underbrace{\frac{2\pi}{L} i}_{\Delta k}$$

$$\sum_k f(k) = \frac{L^3}{(2\pi)^3} \sum_k f(k) \underbrace{\frac{(2\pi)^3}{L^3}}_{(\Delta k)^3} = \frac{L^3}{(2\pi)^3} \sum_k f(k)(\Delta k)^3 \qquad \Delta k \to 0$$

$$\Delta k \to 0 \Rightarrow$$

$$\sum_k f(k) \longrightarrow \frac{L^3}{(2\pi)^3} \int_k f(k) d^3k$$

$$d = 1, 2, 3$$

$$\sum_k f(k) = \textcircled{2} \frac{L^d}{(2\pi)^d} \int_k f(k) (dk)^d$$

degeneracy of the spin