FYS3110 Oblig 3

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1 Problem 3

1.1 a)

The Hamiltonian of the system is:

$$\hat{H} = -g \sum_{i=0}^{N-1} \Big(|i\rangle \langle i+1| + |i+1\rangle \langle i| \Big) - V |0\rangle \langle 0| \tag{1}$$

We set $N = 4$ and write down the matrix representation of the Hamiltonian in the basis where $\langle 0| \simeq \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ and $\langle 1| \simeq \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ etc.

First we write it out with our value for N

$$\hat{H} = -g \sum_{i=0}^{3} \Big(|i\rangle \langle i+1| + |i+1\rangle \langle i| \Big) - V |0\rangle \langle 0| \tag{2}$$

$$\hat{H} = -g\Big(|0\rangle \langle 1| + |1\rangle \langle 0| + |1\rangle \langle 2| + |2\rangle \langle 1| + |2\rangle \langle 3| + |3\rangle \langle 2| + |3\rangle \langle 4| + |4\rangle \langle 3| \Big) - V |0\rangle \langle 0| \tag{3}$$

Writing this out using the basis vectors from earlier we get:

$$\hat{H} = -g \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} - \begin{pmatrix} V & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4}$$

Which gives us:

$$\hat{H} = -g \begin{pmatrix} V/g & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{5}$$

1.2 b)

For this problem we need to find a matrix representing the position operator $\hat{X}$. We know that the eigenvalues represent the atom at which our electron is localized. We choose $N = 4$ giving us the eigenvalues $\Lambda = 0, 1, 2, 3$. From this we can calculate our matrix using the orthonormality of the eigenkets.

$$\langle 0|\hat{X}|0\rangle = 0,\ \langle 1|\hat{X}|1\rangle = 1,\ \langle 2|\hat{X}|2\rangle = 2,\ \langle 3|\hat{X}|3\rangle = 3 \tag{6}$$

from $\langle i|\,|j\rangle = 1$ if $i = j$ and $\langle i|\,|j\rangle = 0$ if $i \neq j$ This results i the matrix

$$\hat{X} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \tag{7}$$

1.3 c)

For this exercise we need to numerically generate our matrix using the given values of $N = 32, g = 1$ and $V = 4$ with our expression for the Hamiltonian (eq.(1)).

```
from numpy import *
from numpy.linalg import *
from matplotlib.pyplot import *
g = 1
V = 4
N = 32
basis = []
for i in range(N):
        b = zeros(N)
        b[i] = 1
        b = matrix(b).T
        basis.append(b)


H = zeros((N,N))
for i in range(N-1):
        H = H -g*(basis[i]*basis[i+1].T+basis[i+1]*basis[i].T) #summing values 0 to N
H = H -g*(basis[-1]*basis[0].T+basis[0]*basis[-1].T) #Making sure i+1=N=0
H = H-V*(basis[0]*basis[0].T) #Adding potential

plot(range(N), sort(eigvals(H)))
title('Eigenvalue diagram')
ylabel('Value eigenvalue')
show()

print H
print eigvals(H)
print "The lowest eigenvalue is Lambda= %.3f" % min(eigvals(H))
```

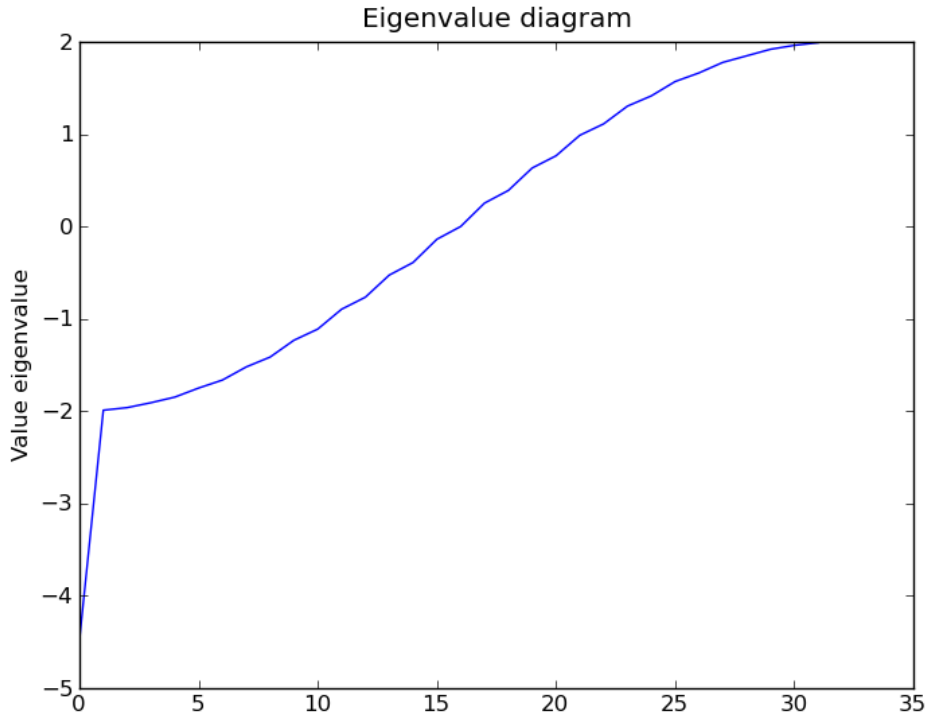

Figure 1: Eigenvalues from min to max

From figure 1 we can gather that the lowest energy is equal to the lowest eigenvalue $\Lambda = -4.472$ as well as from the code printout:

```
[[-4. -1.  0. ...,  0.  0. -1.]
 [-1.  0. -1. ...,  0.  0.  0.]
 [ 0. -1.  0. ...,  0.  0.  0.]
 ...,
 [ 0.  0.  0. ...,  0. -1.  0.]
 [ 0.  0.  0. ..., -1.  0. -1.]
 [-1.  0.  0. ...,  0. -1.  0.]]
[ -4.47213595e+00  -1.98974034e+00   1.99094261e+00   1.91888827e+00
   1.77695753e+00  -1.90841083e+00  -1.74964538e+00   1.56957610e+00
  -1.52082662e+00   1.30348176e+00  -1.23218869e+00   9.87690606e-01
  -8.96133295e-01   6.33313168e-01  -5.26587138e-01   2.53221011e-01
  -1.38402808e-01   1.96157056e+00  -1.96157056e+00   1.84775907e+00
   1.66293922e+00  -1.84775907e+00   1.41421356e+00  -1.66293922e+00
  -1.41421356e+00  -1.11114047e+00   1.11114047e+00  -7.65366865e-01
   7.65366865e-01   2.10317280e-17   3.90180644e-01  -3.90180644e-01]
The lowest eigenvalue is Lambda= -4.472
```

1.4 d)

For this exercise we need to calculate the probability of findig the electron when N=0 and N=1. This is given by $c_n = \langle f_n | \Psi \rangle$ Our probability is given by $|c_n|^2$ which follows from the normalization of the wave function. Finding these probabilities using python and our previous script is done by adding:

```
eigenvalues, eigenvectors = eig(H)
print abs(eigenvectors[0,0])**2
print abs(eigenvectors[1,0])**2
```

Which prints:

```
0.894427191
0.0498447189992
```

So the probabilites corresponding to atom N=0 and N=1 are 89.44% and 4.98%

1.5 e)

To find the ground state expectation value $\langle \psi | \hat{X} | \psi \rangle$ we need to find the sum over all possible outcomes of the eigenvalue times the probability of getting that eigenvalue.

```
X = diag(range(N))
eigenvalues, eigenvectors = eig(H)
print eigenvectors[0]*X*eigenvectors[0].T
```

This prints our expectation value: [[1.20804923]]