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FYS3110 - Quantum Mechanics

Oblig 03

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1 Introduction

Motivate the reader Very often we are ending with a differential equation after solving a mathematical problem, for example Poisson's equation from electromagnetism. –I may should put a little historical review here–. Therefore they made some good analytical methods for solving this kind of equations, but what do we do if we need to solve this numerical?

a)

I will in this exercise find a matrix-representation of the Hamiltonian. This could be done for a general n (I have done it numerical, see exercise c)), but here I will find the 4×4 matrix just to spare some space. Then we have

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

$$= -g \Big(|0\rangle \langle 1| + |1\rangle \langle 0| + |1\rangle \langle 2| + |2\rangle \langle 1| + |2\rangle \langle 3| + |3\rangle \langle 2| \Big) - V |0\rangle \langle 0|$$

$$= -g \Bigg(\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$+ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \Bigg) - V \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\underline{\hat{H} = -q \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} - V \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}$$

This is as we expect, the outer products give matrices, and we and up with to terms. In general a Hamiltonian consists of a kinetic energy term and a potential term, so the expression found above matches with this.

b)

Here we shall find a representation for the position operator. We already know that it should have the atom indexes as eigenvalues, and the basis should be the same as in the previous exercise. We obtain

$$\hat{X} |0\rangle = 0 |0\rangle \quad \Rightarrow \quad \hat{X} |i\rangle = i |i\rangle$$

so mathematical we can write this as

$$x_{11} = 0, \quad x_{22} = 1, \quad ... \quad x_{ii} = (i-1)$$

NB! Notice that this is the mathematical implementation, numerical we will shift the indexes, so we will have $x_{ii} = i$

Therefore the matrix-representation for the position operator is

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

when $n = 4$

c)

When we are measuring energy, the only results we can have is the eigenvalues of $\hat{H}$. Therefore the lowest energy we can measure is the lowest (the first) eigenvalue, which has value -4.25. The energy diagram looks like this (*see Figure 1*): *I have calculated this numerical in Python, please see the appendix in the back of this assignment to find the code attachment.*

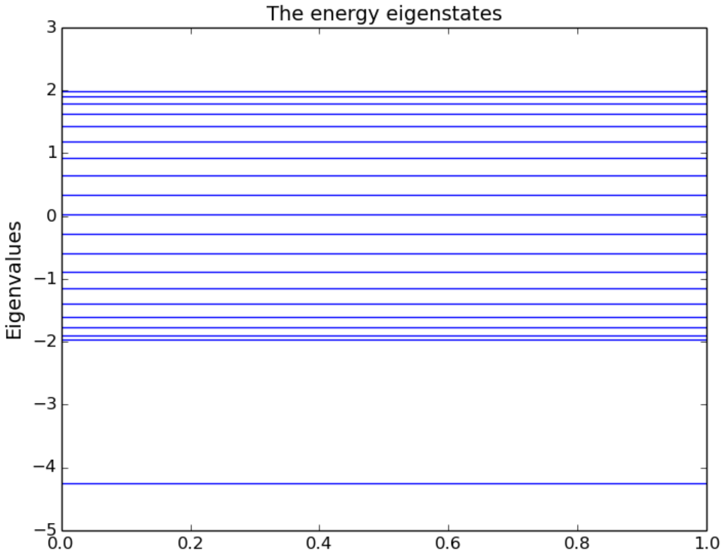

Figure 1: The energy eigenstates for $n = 20$.

d)

The Born rule states that

$$P(x) = |\Psi(x)|^2$$

where $\Psi(x) = \langle x|\psi(x)\rangle$. In our case, I find that

$$P_g(0) = |\langle 0|\psi_g\rangle|^2 \cong 0.9375$$

$$P_g(1) = |\langle 1|\psi_g\rangle|^2 \cong 0.0586$$

Where $P_g(i)$ is the probability to find the electron by atom i in the ground state. I have done the calculations numerical.

e)

We know that the expectation value for position is given by

$$\langle x\rangle_g = \langle\psi_g|\hat{X}|\psi_g\rangle$$

where ψ_g is the ground state. We can split this up to two inner products:

$$\left\langle \psi_g \middle| \left\langle \hat{X} \middle| \psi_g \right\rangle \right\rangle$$

or just

$$a = \left\langle \hat{X} \middle| \psi_g \right\rangle, \quad \langle x\rangle_g = \langle\psi_g|a\rangle$$

I have implemented this in my program, and got that the

$$\underline{\langle x\rangle \approx \frac{2}{3}}$$

Physical this is the place between atom 0 and atom 1, but note: There is not possible to measure this value! The electron will always be bound to a specific atom, and the expectation value is just a average over all the possible states.

f)

In this exercise I will assume that the electron is attracted at atom 0 in the beginning. Then we will calculate the probability to find the electron on the same atom at a later time. First we know that atom 0 can be expressed as

$$|0\rangle = \sum_n C_n |E_n\rangle$$

The easiest way to find the probability at a later time is to use the propagator $\hat{U}$:

$$\hat{U}|0\rangle = \hat{U}\sum_n Cn|E_n\rangle = C_n e^(- iE_n t/\hbar)|E_n\rangle$$

So the probability should be

$$P(t,0) = \sum_{n=1}^{N-1} C_n e^(-iE_n t/\hbar) |E_n\rangle$$

When I do this numerical, I get this plot:

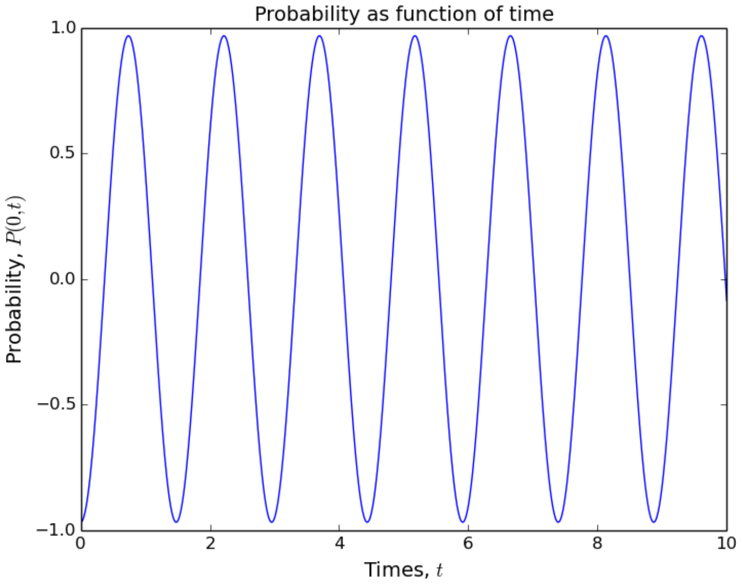

Figure 2: The energy eigenstates for $n = 20$.

I know this is not the right solution, the real solution should not be harmonic. I guess is something wrong with my analytical expression.

Code attachment

Here is the code that I have used in this problem set:

```
import numpy as np
import matplotlib.pyplot as plt
from numpy.linalg import eigh

#Constants
g=1
V=4
N=20
M=1000
hbar=1
```

```
comp=1.j

#Matrices
I=np.identity(N)      # Taking columns from I
A=np.zeros([N,N])     # A is the outer product
A[0,0]=1              # |0><0|

#Hamiltonian (Exercise C)
gpart=0
for i in range(N-1):
    gpart+=np.outer(I[i],I[i+1])+np.outer(I[i+1],I[i])
H=g*gpart-V*A
[eigvals,eigmat]=eigh(H) # Gives the eigenvalues and
                         # eigenvectors of a hermitian
#print "The eigenvalues are: ",eigvals
#print "The eigenvectors are: ",eigmat

#Exercise D
P=np.zeros(N)
for i in range(N):
    P[i] = (np.inner(I[i],eigmat[:,0]))**2
print "P_g(0) = ",P[0]
print "P_g(1) = ",P[1]

#Exercise E
X=np.zeros([N,N])
for i in range(N):
    X[i,i]=i
a=np.inner(X,eigmat[:,0])
b=np.inner(eigmat[:,0],a)
print "The expectation value is: ",b

#Exercise F
C=np.zeros([M,N])
c_start=np.zeros(N)
tlist=np.linspace(0,10,M)

for i in range(N):
    c_start[i]=np.inner(I[0],eigmat[:,i])

for i in range(M):
    for j in range(N):
        C[i,j]=c_start[j]*np.exp(eigvals[j]*tlist[i]*comp/hbar)

#Plot
SZ={’size’:’14’}         #Size of label
for value in eigvals:
    plt.axhline(value)   #Plot hor. line for eigenvalues
plt.axis([0,1,-5,3])     #Set axis
plt.title(’The energy eigenstates’,**SZ)
plt.ylabel(’Eigenvalues’,**SZ)
plt.show()

plt.title(’Probability as function of time’,**SZ)
plt.xlabel(’Times, $t$’,**SZ)
plt.ylabel(’Probability, $P(0,t)$’,**SZ)
plt.plot(tlist,C[:,0])
plt.show()
```

Right now this program gives the print:

```
P_g(0) = 0.9375
P_g(1) = 0.05859375
The expectation value is: 0.0666666666667
```