Ejercicio 3.2

Se supone que $n_g = 0$ y $e_J = 50$. El Hamiltoniano truncado, con $N = 2$, y los vectores propios se calculan con el siguiente programa.

```
import numpy as np
from numpy import linalg

N = 2
ng = 0
eJ = 50

def resetH(N):
    return np.zeros((2*N+1, 2*N+1))
def setH(N, ng, eJ):
    MH = resetH(N)
    for i in range(2*N+1):
        MH[i,i] = 4*((i-N-ng)**2)
    for i in range(1,2*N+1):
        MH[i-1,i] = -0.5*eJ
    for i in range(2*N):
        MH[i+1,i] = -0.5*eJ
    return MH

def eigen_vectors(N,ng,eJ):
    M = setH(N,ng,eJ)
    vector_list = linalg.eig(M)[1]
    for i in range(2*N+1):
        V = [vector_list[0,i]]
        for j in range(2*N):
            V = V+[vector_list[j+1,i]]
        P = M@V
        Q = P/V
        print("eigen_vector(",i,")=", V)
        print("eigen_value(",i,")=",Q[0])
        print("================================================================")

eigen_vectors(N,ng,eJ)
H = setH(N, ng, eJ)
```

Este es el resultado.

```
eigen_vector( 0 )= [-0.2253978360612247, -0.49772406702680333, -0.6347701451725904, -
0.4977240670268029, -0.2253978360612244]
eigen_value( 0 )= -39.205062715376606
================================================================
eigen_vector( 1 )= [0.4377862056771192, 0.5552866269944118, 8.241172092603234e-18, -
0.5552866269944119, -0.4377862056771194]
eigen_value( 1 )= -15.709920264364884
================================================================
eigen_vector( 2 )= [0.5576465182758401, 0.12342013749550008, -0.5895724388324555,
0.12342013749550036, 0.5576465182758404]
eigen_value( 2 )= 10.466918852237402
================================================================
eigen_vector( 3 )= [-0.3717878106578396, 0.486865713275118, -0.4994709222434463,
0.48686571327511957, -0.3717878106578417]
eigen_value( 3 )= 48.73814386313931
================================================================
eigen_vector( 4 )= [-0.555286626994412, 0.4377862056771198, -8.300428695993057e-16, -
0.43778620567711884, 0.5552866269944116]
eigen_value( 4 )= 35.709920264364904
================================================================
```

Por tanto, definiendo las listas v_0, v_1, v_2, v_3, v_4,

```
v0 = [-0.2253978360612247, -0.49772406702680333, -0.6347701451725904, -
0.4977240670268029, -0.2253978360612244]

v1 = [0.4377862056771192, 0.5552866269944118, 8.241172092603234e-18, -
0.5552866269944119, -0.4377862056771194]

v2 = [0.5576465182758401, 0.12342013749550008, -0.5895724388324555, 0.12342013749550036,
0.5576465182758404]
```

```
v3 = [-0.555286626994412, 0.4377862056771198, -8.300428695993057e-16, -
0.43778620567711884, 0.5552866269944116]

v4 = [-0.3717878106578396, 0.486865713275118, -0.4994709222434463, 0.48686571327511957,
-0.3717878106578417]
```

los estados propios, en la base de los estados de carga, son

$|\psi_0\rangle = v_0[0]\,|-2\rangle + v_0[1]|-1\rangle + v_0[2]|0\rangle + v_0[3]|1\rangle + v_0[4]|2\rangle,$
$|\psi_1\rangle = v_1[0]\,|-2\rangle + v_1[1]|-1\rangle + v_1[2]|0\rangle + v_1[3]|1\rangle + v_1[4]|2\rangle,$
$|\psi_2\rangle = v_2[0]\,|-2\rangle + v_2[1]|-1\rangle + v_2[2]|0\rangle + v_2[3]|1\rangle + v_2[4]|2\rangle,$
$|\psi_3\rangle = v_3[0]\,|-2\rangle + v_3[1]|-1\rangle + v_3[2]|0\rangle + v_3[3]|1\rangle + v_3[4]|2\rangle,$
$|\psi_4\rangle = v_4[0]\,|-2\rangle + v_4[1]|-1\rangle + v_4[2]|0\rangle + v_4[3]|1\rangle + v_4[4]|2\rangle.$

Se puede comprobar que son ortonormales. El programa siguiente

```
acc = 0
for i in range(5):
    acc = acc + v0[i]**2
print("(v0,v0) = ", acc)

...

acc = 0
for i in range(5):
    acc = acc + v3[i]*v4[i]
print("(v3,v4) = ", acc)
```

genera los diferentes productos internos

```
(v0,v0) =  1.0
(v1,v1) =  1.0
(v2,v2) =  0.9999999999999998
(v3,v3) =  1.0
(v4,v4) =  0.9999999999999998

(v0,v1) =  -2.498001805406602e-16
(v0,v2) =  -2.7755575615628914e-16
(v0,v3) =  1.3877787807814457e-16
(v0,v4) =  1.249000902703301e-16
(v1,v2) =  -4.163336342344337e-16
(v1,v3) =  8.326672684688674e-17
(v1,v4) =  1.1102230246251565e-16
(v2,v3) =  4.440892098500626e-16
(v2,v4) =  -1.1102230246251565e-16
(v3,v4) =  -8.604228440844963e-16
```

con pequeñas imprecisiones de cálculo.

Redondeando, se obtiene la siguiente representación de los estados propios en la base de los estados de carga:

$|\psi_0\rangle = -0.225|-2\rangle - 0.498|-1\rangle -0.635|0\rangle - 0.498|1\rangle - 0.225|2\rangle,$
$|\psi_1\rangle = 0.438|-2\rangle + 0.555|-1\rangle \quad -0.555|1\rangle - 0.438|2\rangle,$
$|\psi_2\rangle = 0.558|-2\rangle + 0.123|-1\rangle - 0.59|0\rangle + 0.123|1\rangle + 0.558|2\rangle,$
$|\psi_3\rangle = -0.555|-2\rangle + 0.438|-1\rangle \quad -0.438|1\rangle + 0.555|2\rangle,$
$|\psi_4\rangle = -0.372|-2\rangle + 0.487|-1\rangle - 0.5\,|0\rangle + 0.487|1\rangle - 0.372|2\rangle.$

Ejercicio 3.3

La matriz *M* que transforma los coeficientes de un vector representado en la base de los estados de carga en su representación en la base de los estados propios es la siguiente:

```
M = np.matrix([v0, v1, v2, v3, v4]).transpose()
print("M = ", M)

M =  [[-2.25397836e-01  4.37786206e-01  5.57646518e-01 -5.55286627e-01
  -3.71787811e-01]
 [-4.97724067e-01  5.55286627e-01  1.23420137e-01  4.37786206e-01
   4.86865713e-01]
 [-6.34770145e-01  8.24117209e-18 -5.89572439e-01 -8.30042870e-16
  -4.99470922e-01]
 [-4.97724067e-01 -5.55286627e-01  1.23420137e-01 -4.37786206e-01
   4.86865713e-01]
 [-2.25397836e-01 -4.37786206e-01  5.57646518e-01  5.55286627e-01
  -3.71787811e-01]]
```

Se comprueba que la matriz *M* es unitaria (con pequeñas imprecisiones de cálculo).

```
print("M@MT = ", M @ M.transpose())

M@MT =  [[ 1.00000000e+00  4.43308766e-16  2.58813124e-16  2.81768058e-16
   1.13715180e-16]
 [ 4.43308766e-16  1.00000000e+00  2.91483260e-16 -1.14320863e-16
  -1.11852545e-16]
 [ 2.58813124e-16  2.91483260e-16  1.00000000e+00 -2.07294749e-16
  -1.98586809e-17]
 [ 2.81768058e-16 -1.14320863e-16 -2.07294749e-16  1.00000000e+00
  -2.73393254e-16]
 [ 1.13715180e-16 -1.11852545e-16 -1.98586809e-17 -2.73393254e-16
   1.00000000e+00]]
```

Las columnas de M^T, es decir, las filas de *M*, son los coeficientes de la representación de los estados de carga en la base de los estados propios:

$|-2\rangle = v_0[0]\,|\psi_0\rangle + v_1[0]\,|\psi_1\rangle + v_2[0]\,|\psi_2\rangle + v_3[0]\,|\psi_3\rangle + v_4[0]\,|\psi_4\rangle,$
$|-1\rangle = v_0[1]\,|\psi_0\rangle + v_1[1]\,|\psi_1\rangle + v_2[1]\,|\psi_2\rangle + v_3[1]\,|\psi_3\rangle + v_4[1]\,|\psi_4\rangle,$
$|0\rangle = v_0[2]\,|\psi_0\rangle + v_1[2]\,|\psi_1\rangle + v_2[2]\,|\psi_2\rangle + v_3[2]\,|\psi_3\rangle + v_4[2]\,|\psi_4\rangle,$
$|1\rangle = v_0[3]\,|\psi_0\rangle + v_1[3]\,|\psi_1\rangle + v_2[3]\,|\psi_2\rangle + v_3[3]\,|\psi_3\rangle + v_4[3]\,|\psi_4\rangle,$
$|2\rangle = v_0[4]\,|\psi_0\rangle + v_1[4]\,|\psi_1\rangle + v_2[4]\,|\psi_2\rangle + v_3[4]\,|\psi_3\rangle + v_4[4]\,|\psi_4\rangle.$

Rondeando:

$|-2\rangle = -0.225|\psi_0\rangle + 0.438|\psi_1\rangle + 0.558|\psi_2\rangle - 0.555|\psi_3\rangle - 0.372|\psi_4\rangle,$
$|-1\rangle = -0.498|\psi_0\rangle + 0.555|\psi_1\rangle + 0.123|\psi_2\rangle + 0.438|\psi_3\rangle + 0.487|\psi_4\rangle,$
$|0\rangle = -0.635|\psi_0\rangle - 0.59|\psi_2\rangle - 0.5|\psi_4\rangle,$
$|1\rangle = -0.498|\psi_0\rangle - 0.555|\psi_1\rangle + 0.123|\psi_2\rangle - 0.438|\psi_3\rangle + 0.487|\psi_4\rangle,$
$|2\rangle = -0.225|\psi_0\rangle - 0.438|\psi_1\rangle + 0.558|\psi_2\rangle + 0.555|\psi_3\rangle - 0.372|\psi_4\rangle,$