Ejercicio 3.5.4

Se supone que $n_g = 0$ y $e_J = 50$ y se usa el Hamiltoniano truncado con $N = 2$. 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)
```

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, ordenadas de acuerdo con los valores propios correspondientes, es decir,

```
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]
```

se representan como sigue los estados propios en la base de los estados de carga:

$|\psi_0\rangle = v_0[0]\,|\text{-}2\rangle + v_0[1]|\text{-}1\rangle + v_0[2]|0\rangle + v_0[3]|1\rangle + v_0[4]|2\rangle,$

$|\psi_1\rangle = v_1[0]\,|\text{-}2\rangle + v_1[1]|\text{-}1\rangle + v_1[2]|0\rangle + v_1[3]|1\rangle + v_1[4]|2\rangle,$

$|\psi_2\rangle = v_2[0]\,|\text{-}2\rangle + v_2[1]|\text{-}1\rangle + v_2[2]|0\rangle + v_2[3]|1\rangle + v_2[4]|2\rangle,$

$|\psi_3\rangle = v_3[0]\,|\text{-}2\rangle + v_3[1]|\text{-}1\rangle + v_3[2]|0\rangle + v_3[3]|1\rangle + v_3[4]|2\rangle,$

$|\psi_4\rangle = v_4[0]\,|\text{-}2\rangle + v_4[1]|\text{-}1\rangle + v_4[2]|0\rangle + v_4[3]|1\rangle + v_4[4]|2\rangle.$

La matriz de transformación de la base de los vectores propios a la base de los estados de carga es

$M = [M_{kl}] = v_k[l].$

El programa siguiente define M y comprueba que $MM^T = I$, confirmándose así que $\{|\psi_0\rangle, \ldots, |\psi_4\rangle\}$ y $\{|\text{-}2\rangle, \ldots, |2\rangle\}$ son bases ortonormales:

```
import numpy as np
from numpy import linalg
M = np.matrix([v0, v1, v2, v3, v4])
MT = M.transpose()
print(M@MT)
```

Este es el resultado :

```
[[ 1.00000000e+00 -2.62200282e-16 -2.50312345e-16  1.37569117e-16
   1.03044105e-16]
 [-2.62200282e-16  1.00000000e+00 -4.56714042e-16  8.60130738e-17
   8.41811740e-17]
 [-2.50312345e-16 -4.56714042e-16  1.00000000e+00  4.24853240e-16
  -1.15733514e-16]
 [ 1.37569117e-16  8.60130738e-17  4.24853240e-16  1.00000000e+00
  -8.07730940e-16]
 [ 1.03044105e-16  8.41811740e-17 -1.15733514e-16 -8.07730940e-16
   1.00000000e+00]]
```

Es la matriz unidad 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$|-1\rangle$ -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$|-1\rangle$ -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 3.5.5

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

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

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

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

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

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

Redondeando:

$|-2\rangle = -0.225|\psi_0\rangle + 0.438|\psi_1\rangle + 0.558|\psi_2\rangle - 0.555|\psi_3\rangle - 0.372|\psi_4\rangle,$

$|-1\rangle = -0.498|\psi_0\rangle + 0.555|\psi_1\rangle + 0.123|\psi_2\rangle + 0.438|\psi_3\rangle + 0.487|\psi_4\rangle,$

$|0\rangle = -0.635|\psi_0\rangle - 0.59|\psi_2\rangle - 0.5|\psi_4\rangle,$

$|1\rangle = -0.498|\psi_0\rangle - 0.555|\psi_1\rangle + 0.123|\psi_2\rangle - 0.438|\psi_3\rangle + 0.487|\psi_4\rangle,$

$|2\rangle = -0.225|\psi_0\rangle - 0.438|\psi_1\rangle + 0.558|\psi_2\rangle + 0.555|\psi_3\rangle - 0.372|\psi_4\rangle.$

Ejercicio 3.5.6

Como en los ejercicios anteriores se supone que $n_g = 0$ y $e_J = 50$, pero se usa el Hamiltoniano truncado con $N = 1$. Los vectores propios se calculan con el mismo programa programa que en el ejercicio 3.5.4 cambiando el valor de N:

```
eigen_vector( 0 )= [0.48567523884986946, 0.7268006086515374,
0.4856752388498689]
eigen_value( 0 )= -33.41186241925151
================================================================
eigen_vector( 1 )= [-0.7071067811865475, -1.6969347377467985e-16,
0.7071067811865475]
eigen_value( 1 )= 3.999999999999994
================================================================
eigen_vector( 2 )= [0.5139256389480122, -0.6868485096902772,
0.5139256389480124]
eigen_value( 2 )= 37.41186241925155
================================================================
```

Por tanto, redondeando,

$|\psi_0\rangle = 0.486|\text{-}1\rangle + 0.727|0\rangle + 0.486|1\rangle$,

$|\psi_1\rangle = \text{-}0.707|\text{-}1\rangle + 0.707|1\rangle$,

$|\psi_2\rangle = 0.514|\text{-}1\rangle - 0.687|0\rangle + 0.514|1\rangle$,

y

$|\text{-}1\rangle = 0.486|\psi_0\rangle - 0.707|\psi_1\rangle + 0.514|\psi_2\rangle$,

$|0\rangle = \text{-}0.727|\psi_0\rangle - 0.687|\psi_2\rangle$,

$|1\rangle = \text{-}0.486|\psi_0\rangle + 0.707|\psi_1\rangle + 0.514|\psi_2\rangle$.

Los valores relativos de la energía, es decir, los valores propios del Hamiltoniano, son

$E_0/E_C = \text{-}33.4$, $E_1/E_C = 4$, $E_2/E_C = 37.4$.

Las frecuencias angulares correspondientes son

$\omega_0 = E_0/\hbar, = \text{-}33.4E_C/\hbar$, $\omega_1 = E_1/\hbar, = 4E_C/\hbar$, $\omega_2 = E_2/\hbar, = 37.4E_C/\hbar$,

es decir,

$\omega_0 = \text{-}33.4\omega_C$, $\omega_1 = 4\omega_C$, $\omega_2 = 37.4\omega_C$, con $\omega_C = E_C/\hbar$.

El operador unitario que describe la evolución del sistema es, según (2.45),

$\widehat{U} = e^{i33.4\omega_C\Delta t}|\psi_0\rangle\langle\psi_0| + e^{-i4\omega_C\Delta t}|\psi_1\rangle\langle\psi_1| + e^{-i37.4\omega_C\Delta t}|\psi_2\rangle\langle\psi_2|$.

Por tanto

$\widehat{U}|0\rangle = -0.727\widehat{U}|\psi_0\rangle - 0.687\widehat{U}|\psi_2\rangle$

$= -0{,}727e^{i33.4\omega_C\Delta t}|\psi_0\rangle - 0{,}687e^{-i37.4\omega_C\Delta t}|\psi_2\rangle$.

Obviando el desfase global, se expresa como sigue la evolución del sistema puesto inicialmente en el estado de carga $|0\rangle$:

$\widehat{U}|0\rangle \equiv -0.727|\psi_0\rangle - 0.687e^{-i70.8\omega_C\Delta t}|\psi_2\rangle$

$= -0.727(0.486|-1\rangle + 0.727|0\rangle + 0.486|1\rangle) - 0.687e^{-i70.8\omega_C\Delta t}(0.514|-1\rangle$

$- 0.687|0\rangle + 0.514|1\rangle)$.

Se analiza para diferentes valores de Δt:

- con $\Delta t = 2k\pi/70.8\omega_C$, es decir, $e^{-i70.8\omega_C\Delta t} = 1$,

  $\widehat{U}|0\rangle = -0{,}706|-1\rangle - 0.057|0\rangle - 0{,}706|1\rangle$;

- con $\Delta t = (2k+0.5)\pi/70.8\omega_C$, es decir, $e^{-i70.8\omega_C\Delta t} = i$,

  $\widehat{U}|0\rangle = -(0.353 + 0{,}353i)|-1\rangle - (0.529 - 0.472i)|0\rangle - (0.353 + 0{,}353i)|1\rangle$;

- con $\Delta t = ((2k+1)\pi/70.8\omega_C$, es decir, $e^{-i70.8\omega_C\Delta t} = -1$,

  $\widehat{U}|0\rangle = -|0\rangle$;

- con $\Delta t = (2k+1.5)\pi/70.8\omega_C$, es decir, $e^{-i70.8\omega_C\Delta t} = -i$,

  $\widehat{U}|0\rangle = -(0.353 - 0{,}353i)|-1\rangle - (0.529 + 0.471i)|0\rangle - (0.353 - 0{,}353i)|1\rangle$.

Con las siguientes aproximaciones

$0.706 \approx \frac{1}{\sqrt{2}}$, $0.353 \approx \frac{1}{2\sqrt{2}}$,

se obtienen las siguientes relaciones:

$\widehat{U}|0\rangle \approx \frac{1}{\sqrt{2}}(|-1\rangle + |1\rangle)$ si $\Delta t = 2k\pi/70.8\omega_C$,

$\widehat{U}|0\rangle \approx -\frac{1+i}{2\sqrt{2}}|-1\rangle - \frac{1-i}{2}|0\rangle - \frac{1+i}{2\sqrt{2}}|1\rangle$ si $\Delta t = (2k+0.5)\pi/70.8\omega_C$,

$\widehat{U}|0\rangle \approx -|0\rangle$ si $\Delta t = (2k+1)\pi/70.8\omega_C$,

$\widehat{U}|0\rangle \approx -\frac{1-i}{2\sqrt{2}}|-1\rangle - \frac{1+i}{2}|0\rangle - \frac{1-i}{2\sqrt{2}}|1\rangle$ si $\Delta t = (2k+1.5)\pi/70.8.8\omega_C$.

En términos de probabilidades:

$\Delta t = 2k\pi/70.8\omega_C$: $p(0) = 0$, $p(-1) = p(1) = 0.5$,

$\Delta t = (2k+0.5)\pi/70.8\omega_C$: $p(0) = 0.5$, $p(-1) = p(1) = 0.25$,

$\Delta t = (2k+1)\pi/\ 70.8\omega_C$: $p(0) = 1$, $p(-1) = p(1) = 0$,

$\Delta t = (2k+1.5)\pi/\ 70.8\omega_C$: $p(0) = 0.5$, $p(-1) = p(1) = 0.25$.

Gráficos : $p(k)$ en función de Δt con $T = 2\pi/70.8\omega_C$.