

Ejercicio 3.5.1

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,
-0.5895724388324553, 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:

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

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

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

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

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

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 $\{|\psi_0\rangle, \dots, |\psi_4\rangle\}$ y $\{|-2\rangle, \dots, |2\rangle\}$ 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 3.5.2

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:

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

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

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

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

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

Ejercicio 3.5.3

Como en los ejercicios anteriores se supone que $n_g = 0$ y $e_f = 50$, pero se usa el Hamiltoniano truncado con $N = 1$. Los vectores propios se calculan con el mismo programa programa que en el ejercicio 3.5.1 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 )= 3.9999999999999994  
=====  
eigen_vector( 2 )= [0.5139256389480122, -0.6868485096902772,  
0.5139256389480124]  
eigen_value( 2 )= 37.41186241925155  
=====
```

Por tanto, redondeando,

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

$$|\psi_1\rangle = -0.707|-1\rangle + 0.707|1\rangle,$$

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

y

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

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

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

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

$$E_0/E_C = -33.4, E_1/E_C = 4, E_2/E_C = 37.4.$$

Las frecuencias angulares correspondientes son

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

es decir,

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

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

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

Por tanto

$$\begin{aligned}\hat{U}|0\rangle &= -0.727\hat{U}|\psi_0\rangle - 0.687\hat{U}|\psi_2\rangle \\ &= -0.727e^{i33.4\omega_c\Delta t}|\psi_0\rangle - 0.687e^{-i37.4\omega_c\Delta t}|\psi_2\rangle.\end{aligned}$$

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

$$\begin{aligned}\hat{U}|0\rangle &\equiv -0.727|\psi_0\rangle - 0.687e^{-i70.8\omega_c\Delta t}|\psi_2\rangle \\ &= -0.727(0.486|-1\rangle + 0.727|0\rangle + 0.486|1\rangle) - 0.687e^{-i70.8\omega_c\Delta t}(0.514|-1\rangle \\ &\quad - 0.687|0\rangle + 0.514|1\rangle).\end{aligned}$$

Se analiza para diferentes valores de Δt :

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

$$\hat{U}|0\rangle = -0.706|-1\rangle - 0.057|0\rangle - 0.706|1\rangle;$$
- con $\Delta t = (2k+0.5)\pi/70.8\omega_c$, es decir, $e^{-i70.8\omega_c\Delta t} = i$,

$$\hat{U}|0\rangle = -(0.353 + 0.353i)|-1\rangle - (0.529 - 0.472i)|0\rangle - (0.353 + 0.353i)|1\rangle;$$
- con $\Delta t = ((2k+1)\pi/70.8\omega_c$, es decir, $e^{-i70.8\omega_c\Delta t} = -1$,

$$\hat{U}|0\rangle = -|0\rangle;$$
- con $\Delta t = (2k+1.5)\pi/70.8\omega_c$, es decir, $e^{-i70.8\omega_c\Delta t} = -i$,

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

Con las siguientes aproximaciones

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

se obtienen las siguientes relaciones:

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

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

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

$$\hat{U}|0\rangle \approx -\frac{1-i}{2\sqrt{2}}|-1\rangle - \frac{1+i}{2}|0\rangle - \frac{1-i}{2\sqrt{2}}|1\rangle \text{ si } \Delta t = (2k+1.5)\pi/70.8\omega c.$$

En términos de probabilidades:

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

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

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

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