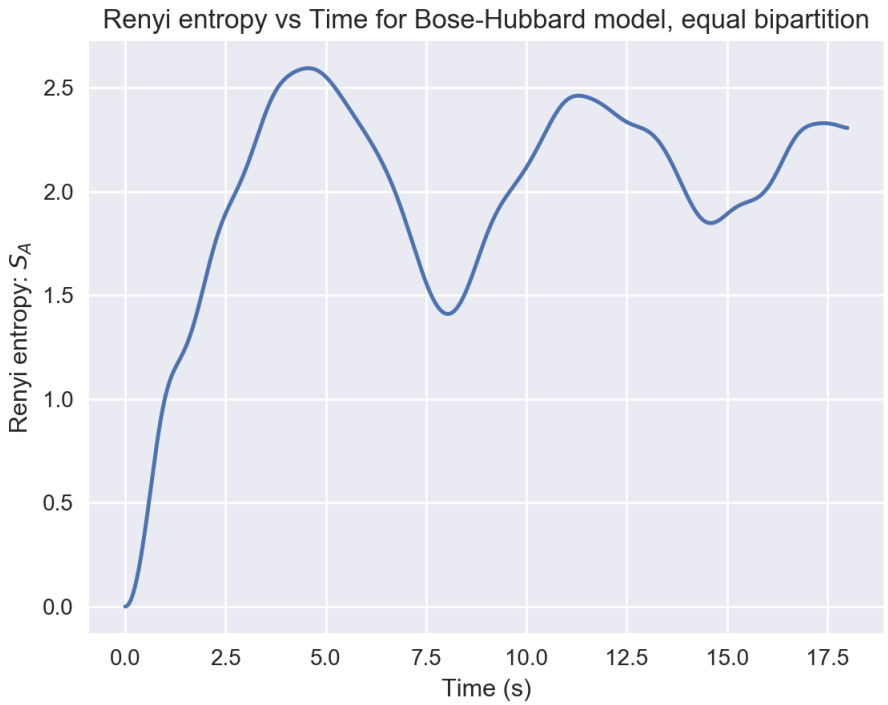
Quantum Many Body Physics – Final Report

This is the report for Question 3 of the final project.
Simulation of the Bose-Hubbard model for a system of 6 bosons, equally bipartitioned.
The parameters are J = 0.64, U = 1, N=M=6
The initial state is: |111111>

For this system, the 4 lowest energies are:

-2.73365543	-2.19555066	-1.85501885	-1.73438068

The resultant plot for Renyi entropy over time is:



See overleaf for code. Comments. Docstrings & multi-line text. Classes & functions. Builtins & keywords.

```python
# -*- coding: utf-8 -*-
"""
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python script to complete final project of Quantum Many-Body Physics module
Simulate experiment by Kaufman et al. 2016

Python version: 3.5.4
"""

from scipy.special import factorial as fact
import scipy as sp
import numpy as np
import itertools
from copy import deepcopy
import matplotlib.pyplot as plt
#import seaborn as sns
#sns.set()

class tColors:
    """
    Color class for debugging
    """
    WARN = '\x1b[93m'
    FAIL = '\x1b[91m'
    ENDC = '\x1b[0m'

class StateObj:
    """
    Class to keep track of state vector, prefactor and type
    idx is a parameter that keeps basis states in the correct order according
    to the integer representation of the vector.
    Includes creation, annihilation and number operators, deepcopy'd to prevent
    modifying basis states.
    """
    # Initialise attributes
    def __init__(self, init_vec, idx, _type):
        if(type(init_vec) != np.ndarray):
            raise TypeError('init_vec should be a numpy.ndarray')
        self.vector = init_vec
        self.idx = idx
        self.type = _type
        self.prefactor = 1
    # Creation operator
    def create(self, index, N):
        trans = deepcopy(state)
        if(trans.vector[index] == N):
            trans.prefactor = 0
        else:
            trans.vector[index] += 1
        return trans
    # Annihilation operator
    def destroy(self, index):
        trans = deepcopy(state)
        if(trans.vector[index] == 0):
            trans.prefactor = 0
        else:
            trans.vector[index] -= 1
        return trans
    # Number operator
    def num(self, index):
        if(self.vector[index] == 0):
            return -1
        return 1

def getBasisStates(N, M):
    """
    Function to get a list of basis states, ordered by the integer
    representation of the state vector.
    """
    x = itertools.product(range(N + 1), repeat=M)
    basis = [np.asarray(i, dtype=int) for i in x if np.sum(i)==N]
    states = np.asarray([StateObj(basis[i], i, 'boson') for i in
                         range(len(basis))])

    return states

def actHam(state, N, J, U):
    """
    Act hamiltonian on a state, as a series of Creation, Annihilation and
    Number operators. Copy states so that the original state is not effected.
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    Multiply by appropriate parameters, J, U.
    Returns an array of new states with appropriate prefactors.
    """
    t1, t2 = [], []
    # First term
    for i in range(len(state.vector)-1):
        t1.append(state.create(i+1, N).destroy(i))
        t1.append(state.create(i, N).destroy(i+1))
    # Second term
    for i in range(len(state.vector)):
        PREFACTOR = (state.num(i)**2) - state.num(i)
        temp3 = deepcopy(state)
        temp3.prefactor *= (PREFACTOR*U/2)
        t2.append(temp3)

    for state in t1:
        state.prefactor *= (-1 * J)

    return np.r_[t1, t2]

def getHamMatrix(N, M, J, U):
    """
    Get hamiltonian matrix by acting hamiltonian on each basis state.
    """
    basis = getBasisStates(N, M)
    ham_matrix = np.zeros((len(basis), len(basis)))
    for state in basis:
        # Act ham on each basis state
        acted = actHam(state, N, J, U)
        for x in acted:
            for b in basis:
                # Find the matrix location of the 'acted' state and enter into
                # Hamiltonian matrix.
                if(np.all(x.vector == b.vector)):
                    ham_matrix[state.idx][b.idx] += x.prefactor
    # Return ham matrix and basis
    return ham_matrix, basis

def getInitialState(N, M, count=0, default=False):
    """
    Get initial state vector from user.
    """
    LENGTH = int((fact(N+M-1))/(fact(N)*fact(M-1)))
    PREAMBLE = """Enter initial state configuration (e.g. "1, 0, 0").
Note: This is the normalised vector representing the superposition of basis
states.
The basis states are ordered in ascending order of their integer representation
e.g. the state (0, 2) -> "2" will be [1, 0, 0], the state (1, 1) -> "11" will
be [0, 1, 0] and the state (2, 0) -> "20" will be [0, 0, 1].
Should have length: C(N+M-1, N) = """ + str(LENGTH) + ': '
    if(default):
        idx = int(LENGTH/2)
        initialStateVec = np.zeros(LENGTH)
        initialStateVec[idx] = 1
        state = StateObj(initialStateVec, None, 'state')

    else:
        initialStateVec = np.asarray([float(x) for x in input(PREAMBLE)
            .split(', ')])
        if(len(initialStateVec) != LENGTH or np.sum(np.square(
                initialStateVec)) != 1.):
            print(tColors.FAIL + '\nLength of initial state should be C(N+M-1,'
                               + 'N)\nState should be normalised.'
                               + tColors.ENDC)
            input('Press Enter to continue...')
            count += 1
            state = getInitialState(N,M,count=count)
        else:
            state = StateObj(initialStateVec, None, 'state')
    return state

def timeEvolve(initialState, hamMatrix, t):
    """
    Evolve a state vector to time t, according to the hamiltonian matrix.
    """
    if(initialState.type == 'boson'):
        raise TypeError('State should not be in boson format.')
    expMat = -1j * hamMatrix * t
    expMat = sp.linalg.expm(expMat)
    vNewState = np.dot(expMat, initialState.vector)
```

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    newState = StateObj(vNewState, None, 'state')
    return newState

def getRDM(state, N, M, basis, ASIZE=1):
    """
    Get reduced density matrix of a state.
    Input state in basis vector representation e.g. [1/sqrt(2), 1/sqrt(2), 0]
    """
    # Every available a state
    a_basis = np.asarray([np.asarray(i) for i in itertools.product(range(N+1),
                          repeat=ASIZE)])
    # Every available b state
    b_basis = np.asarray([np.asarray(i) for i in itertools.product(range(N+1),
                          repeat=(M-ASIZE))])
    # Initialise c_matrix as zeros
    ALEN, BLEN = len(a_basis), len(b_basis)
    c_matrix = np.zeros((ALEN, BLEN), dtype=complex)
    for i in range(len(state.vector)):
        a_vec = basis[i].vector[:ASIZE]
        for j in range(ALEN):
            if(np.all(a_basis[j] == a_vec)):
                a_idx = j
                break
        b_vec = basis[i].vector[ASIZE:]
        for j in range(BLEN):
            if(np.all(b_basis[j] == b_vec)):
                b_idx = j
                break

        c_matrix[a_idx, b_idx] = state.vector[i]

    rdm = np.dot(c_matrix, c_matrix.conj().T)

    return c_matrix, rdm

def entropy(rdm):
    """
    Given a reduced density matrix, return the Renyi entropy
    """
    rdm2 = np.dot(rdm, rdm)
    vals, vecs = sp.linalg.eigh(rdm2)
    _entropy = -np.log(np.sum(vals))
    return _entropy

def getPlot(initDict, tArr):
    """
    Given dictionary of initial parameters and an array of times to evaluate
    at, calculate the Renyi entropy and plot.
    """
    entropy_arr = []
    for t in tArr:
        print('Time: ' + str(t))
        tState = timeEvolve(initDict['initState'], initDict['ham'], t)
        cmat, rdm = getRDM(tState, initDict['N'], initDict['M'],
                           initDict['basis'], initDict['ASIZE'])
        tEntropy = entropy(rdm)
        entropy_arr.append(tEntropy)
    plt.plot(tArr, entropy_arr)
    plt.xlabel('Time (s)')
    plt.ylabel('Renyi entropy: $S_{A}$')
    plt.title('Renyi entropy vs Time for Bose-Hubbard model, equal bipartition')
    #plt.savefig('plot.png', format='png', dpi=100)
    plt.show()
    return

def init():
    """
    Initialisation. Gets parameters from user and construct Hamiltonian matrix.
    Returns dict of params.
    """
    N, M, J, U = [float(x) for x in input(
            'Enter params (comma separated: "N, M, J, U"): ').split(', ')]
    N, M = int(N), int(M)
    default = bool(int(input('Use default initial state? (1, 1, 1...)'
                             + '(yes:1/no:0): ')))
    initialState = getInitialState(N, M, default=default)
    hamMatrix, basis = getHamMatrix(N, M, J, U)
    if(bool(int(input('Print 4 lowest energies? (yes:1, no:0): ')))):
        vals, vecs = sp.linalg.eigh(hamMatrix)
        print(vals[:4])
```

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    ASIZE = int(input('Enter size of A subsystem: '))
    return {'N': N, 'M': M, 'J': J, 'U': U, 'initState': initialState,
            'ham': hamMatrix, 'basis': basis, 'ASIZE': ASIZE}

if(__name__ == '__main__'):
    print('In module.')
    initDict = init()
    getPlot(initDict, np.linspace(0, 18, 801))
```