import time

import os

import sys

from shutil import copyfile

from setup import readInput

from MCCI import performMCCI

start = time.time()

model, nSite, subSpace, nStates, s2Target, maxItr, startSpinTargetItr, energyTola, spinTola, beta, jVal, det, Ms, posibleDet, bondOrder, outputfile, restart, saveBasis = readInput()

newline = ("\nTotal Posible Determinats are %d .\nBreakup are [Ms, No of Determinants] - ")% (sum(posibleDet))

with open (outputfile, "a") as fout:

fout.write(newline)

for i in range(len(Ms)):

newline = ("\t[%d, %d]")%(Ms[i], posibleDet[i])

with open(outputfile, "a") as fout:

fout.write(newline)

if (i+1 == len(Ms)):

fout.write("\n\n")

if ( subSpace > (sum(posibleDet) \*0.8)):

sys.exit("Sub-Space size is more than 80 % of total determinants space. Make Sub-Space size smaller and run it again.\n ")

performMCCI()

newline = ("Total Time Taken in MCCI Calculation is %f sec.")%( time.time() - start )

with open(outputfile, "a") as fout:

fout.write(newline)