UNIVESITY OF ESWATINI
FACULTY OF SCIENCE AND ENGINEERING
DEPARTMENT OF PHYSICS

Examination 2019/2020
COURSE NAME: Compuatational Nanophysics
COURSE CODE: PHY631
TIME ALLOWED: 3 hours

ANSWER ALL QUESTIONS IN SECTION A. CHOOSE ONLY TWO (2) QUESTIONS IN SECTION B.

THIS PAPER IS NOT TO BE OPENED UNTIL PERMISSION HAS BEEN GIVEN BY THE INVIGILATOR.

The exam paper has 19 printed pages, including an Appendix.

Section A

Question 1

(a) Discuss the fundamental differences between a Quantum wire, Quantun well and Quantum dot.

[3 marks]

(b) What happens to the conducting properties, chemical properties and melting point of a semiconducting material when reduced to nano form?

[3 marks]

(c) What is the configuration of Buckminsterfullerene?

[2 marks]

(d) Describe the conductivity of the carbon nanotubes.

[2 marks]

(e) What is magnetoresistance? Discuss its relationship with carbon nanotubes at low temperature.

[3 marks]

(f) Give the four types of Artificial nanomaterial.

[3 marks]

(g) Describe a dendrimer. What are some of its uses?

[2 marks]

(h) Discuss five applications of nanomaterials and the property utilised in each application.

[10 marks]

(i) What is electron confinement (Quantum confinement)?

[2 marks]

Question 2

(a) Describe the following terms

(i) Born-Oppenheimer approximation

[3 marks]

(ii) Potential energy curve/potential energy surface

[3 marks]

(ii) Correlation energy

[3 marks]

(b) What is the variational principle? Explain and give a formula.

[5 marks]

Question 3

(a) Give the two Hohenberg-Kohn theorems.

[8 marks]

(b) What is a local density approximation? What are its limitation?

[6 marks]

(c) Give the advantage and disadvantage of a slater determinant.

[2 marks]

Section B

Question 4

(a) What is a hybrid quantum mechanics/molecular mechanics (QM/MM) method? Describe the different schemes for coupling between the QM and MM parts.

[20 marks]

Question 5

(a) Briefly discuss the following electronic structure methods

(i) Full CI

[4 marks]

(ii) MRCI

[4 marks]

(iii) MCSCF

[4 marks]

(iv) CASSCF

[4 marks]

(v) MP2

[4 marks]

Question 6

In the Appendix you are given a Fortran program, initially written to perfom a ab initio HF calculation for a small two-electron diatomic system. It performs a minimal basis STO-3G calculation for the HeH^+ system. Modify the code to compute the electronic energy for HeH^+ and H_2 range $R = 0.2, 0.4, \ldots, 2.0$ a_0, and $R = 2.5, 3.0, \ldots, 5.0$ a_0. Plot and compare the potential energy curves obtained from the calculations for HeH^+ and H_2 . Submit two sets of programs, one modified for HeH^+ at $R = 5.0$ and the other for H_2 at $R = 5.0$.

[20 marks]

Appendix

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!*********************************************************************
!
!MINIMAL BASIS STO-3G CALCULATION ON HEH+
!
!THIS IS A LITTLE DUMMY MAIN PROGRAM WHICH CALLS HFCALC
!
!APPENDIX B: TWO-ELECTRON SELF-CONSISTENT-FIELD PROGRAM
!OF MODERN QUANTUM CHEMISTRY by
!Attila Szabo and Neil S. Ostlund
! Ed. 2nd (1989) Dover Publications INC.
!
!Labourly Typed by Michael Zitolo (Feb., 2005)
!Edited and Compiled by Michael Zitolo and Xihua Chen
!
!Cleaned up and debugged again by Andrew Long (2012)
!                  and Daniele (kalium) Dondi (2013)
!*********************************************************************

      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      IOP=2
      N=3
      R=1.4632D0
      ZETA1=2.0925D0
      ZETA2=1.24D0
      ZA=2.0D0
      ZB=1.0D0
      CALL HFCALC(IOP,N,R,ZETA1,ZETA2,ZA,ZB)
      END

!*********************************************************************
      SUBROUTINE HFCALC(IOP,N,R,ZETA1,ZETA2,ZA,ZB)
!
!DOES A HARTREE-FOCK CALCULATION FOR A TWO-ELECTRON DIATOMIC
!USING THE 1S MINIMAL STO-NG BASIS SET
!MINIMAL BASIS SET HAS BASIS FUNCTIONS 1 AND 2 ON NUCLEI A AND B
!
!IOP=0 NO PRINTING WHATSOEVER (TO OPTIMIZE EXPONENTS, SAY)
!IOP=1 PRINT ONLY CONVERGED RESULTS
!IOP=2 PRINT EVERY ITERATION
!N STO-NG CALCULATION (N=1,2 OR 3)
!R BONDLENGTH (AU)
!ZETA1 SLATER ORBITAL EXPONENT (FUNCTION 1)
!ZETA2 SLATER ORBITAL EXPONENT (FUNCTION 2)
!ZA ATOMI!NUMBER (ATOM A)
!ZB ATOMI!NUMBER (ATOM B)
!
!*********************************************************************

      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      IF (IOP.EQ.0) GO TO 20
      PRINT 10,N,ZA,ZB
   10 FORMAT(' ',2X,'STO-',I1,'G FOR ATOMI!NUMBERS ',F5.2,' AND
',F5.2//)
   20 CONTINUE
```