CHUKA  **UNIVERSITY**

UNIVERSITY EXAMINATIONS

FIRST YEAR EXAMINATION FOR THE AWARD OF DEGREE OF MSC IN PHYSICS

PHYS 889: ELECTRONIC STRUCTURE OF MATERIALS

STREAMS: MSC PHYSICS Y1 **TIME: 3 HOURS**

DAY/DATE:

INSTRUCTIONS:

- **This paper consists of FIVE Questions, [15 Marks each].**
- **You are required to answer any FOUR Questions out of FIVE**

QUESTION ONE (15 Marks)

a. Using the Hamiltonians for the Hydrogen atom and that of the Helium atom, distinguish between a single electron and many body problem. (8mks)
b. Identify the term in the Hamiltonian in a (i) that results in many body interactions and explain how the Hatree-Fock theory attempted to provide for this interactions. (7 mks)

QUESTION TWO (15 Marks)

Outline the significance of the Bon-Oppenheimer approximation in the solution of the Schrödinger equation, in settings of practical value.

QUESTION THREE (15 Marks)

Silicon is an important element in technology. Like many compound semiconductors, it has a diamond-like crystal structure. Using well labeled illustrations, show the basis axes and atomic positions for the:-

i. Conventional unit cell of the diamond structure (7 mks).
ii. Primitive unit cell of the diamond structure (8 mks)

QUESTION FOUR (15 Marks)

Discuss the role of k points in determining the occupation of the electrons in the irreducible Brillouin zone of a unit cell.

QUESTION FIVE (15 Marks)

Using an element of your choice, write an input script detailing the computational parameters required for calculating the total energy of the system using the Quantum ESPRESSO simulation code.