Ref. No.: Ex/M.Sc./P/II/307/20/2018

MASTER OF SCIENCE EXAMINATION 2018

2nd Year, 1st Semester

CONDENSED MATTER PHYSICS - I

Paper: PHY/TE/307

Time: Two hours **Full marks: 40**

(20 marks for each group).

Use a separate answer-script for each group.

Group A

Answer any **TWO** questions.

1. (a) By using the many-particle antisymmetric wave function

$$\Psi = \frac{1}{\sqrt{N!}}\sum_{P=1}^{N!}(-1)^P P\{u_{\alpha_1}(q_1)u_{\alpha_2}(q_2)\cdots u_{\alpha_N}(q_N)\},$$

show that (i)

$$\langle\Psi|H_1|\Psi\rangle = \sum_i^N \int dq_i\, u^\star_{\alpha_i}(q_i)\, f(q_i)\, u_{\alpha_i}(q_i), \text{ where } H_1 = \sum_i f(q_i), \text{ and } f(q_i) = -\frac{\nabla_i^2}{2} - \frac{1}{r_i},$$

[4]

and (ii)

$$\langle\Psi|H_2|\Psi\rangle = \frac{1}{2}\sum_{j,k}\iint dq_j\, dq_k\, u^\star_{\alpha_j}(q_j)\, u^\star_{\alpha_k}(q_k)\frac{1}{r_{jk}}\left[u_{\alpha_j}(q_j)\, u_{\alpha_k}(q_k) - u_{\alpha_j}(q_k)\, u_{\alpha_k}(q_j)\right].$$

where $H_2 = \frac{1}{2}\sum_{j,k}\frac{1}{r_{jk}}$. Symbols have their usual meaning. [4]

(b) In the Hartree-Fock theory, total energy of an atom (with N electrons) can be expressed as

$$E(N) = \sum_j H_j + \frac{1}{2}\sum_j\sum_{k\neq j} K_{jk} \quad \text{and} \quad H_j = \epsilon_j - \sum_{k\neq j} K_{jk}.$$

Hence prove the Koopmans' theorem, *i. e.*, $E(N) - E(N - i\,th \text{ electron}) = \epsilon_i$. [2]

2. (a) The density function $n(\vec{r})$ is defined as $n(\vec{r}) = \langle\Psi|\hat{n}(\vec{r})|\Psi\rangle$,
where $\hat{n}(\vec{r}) = \sum_{i=1}^N \delta(\vec{r}_i - \vec{r})$. Hence show that

$$n(\vec{r}) = N\int \Psi^\star(\vec{r},\vec{r}_2,\cdots\vec{r}_N)\Psi(\vec{r},\vec{r}_2,\cdots\vec{r}_N)\, d\vec{r}_2\, d\vec{r}_3\cdots d\vec{r}_N.$$

Symbols have their usual meaning. [2]

(b) Show that $n(\vec{r}) = \sum_i |\phi_i(\vec{r})|^2$, when $\Psi = \prod_i \phi_i(\vec{r}_i)$. [1]

(c) For an atom, the external potential energy of the N numbers of interacting electrons due to the nuclear charge (Ze) is given by $(N = Z)$

$$V = \sum_{j=1}^{N} v(\vec{r}_j) \quad \text{where} \quad v(\vec{r}_j) = -\frac{Z}{r_j}.$$

Now show that $\langle\Psi|V|\Psi\rangle = \int v(\vec{r})\, n(\vec{r})\, d\vec{r}$, where
$n(\vec{r}) = N \int \cdots \int |\Psi(\vec{r}, \vec{r}_2, \cdots, \vec{r}_N)|^2\, d\vec{r}_2 \cdots d\vec{r}_N$. [2]

(d) State and prove the Hellmann-Feynman theorem. [2]

(e) The nuclear potential experienced by the electron is given by

$$V = -\sum_i \frac{Z}{r_i},$$

By using the Hellmann-Feynman theorem show that the x-component of the force experienced by the i-th electron is given by

$$F_{ix} = -\frac{\partial \langle V\rangle}{\partial x_i} = \int d\vec{r}_i\, n(\vec{r}_i)\, \frac{Z\, x_i}{r_i^3}.$$

where $\langle V\rangle = \langle\Psi|V|\Psi\rangle$ and Ψ is the ground state wavefunction. [3]

3. (a) Show that a many-particle wave function $\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)$ satisfies the scaling relation $\Psi_\lambda = \lambda^{3N/2}\Psi$. [1]

(b) For a potential that satisfies the relation,

$$V(\lambda\vec{r}_1, \lambda\vec{r}_2, \cdots, \lambda\vec{r}_N) = \lambda^m V(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N),$$

find the scaling relation for $V[\Psi]$. [2]

(c) Find the scaling relation for kinetic energy functional $T[\Psi]$ [2]

(d) By using the Virial theorem in quantum mechanics, find the relation between the kinetic energy (T) and the above potential energy (V) in the ground state. [1]

(e) Suppose the kinetic energy functional $T[\Psi]$ be expressible as $T[n] = \int t(n)\, d\vec{r}$. Find the scaling relation for $t(n)$, *i. e.*, the relation between $t(\lambda n)$ and $t(n)$. [2]

(f) Find the scaling relation for the following exchange energy functional.

$$J[n] = -\frac{1}{8} \int\int \frac{|n(\vec{r}, \vec{r}')|^2}{\vec{r} - \vec{r}'}\, d\vec{r}\, d\vec{r}'.$$

[2]

4. (a) From the first Hohenberg-Kohn theorem develop the Kohn-Sham equations for density functional theory. [4]

(b) Find the expression of total energy functional in terms of Kohn-Sham eigenvalues, ϵ_i and other functionals. [1]

(c) Derive the expression of Dirac exchange energy functional for homogeneous free electron gas. [4]

(d) Describe local density approximation (LDA) on the Dirac exchange energy functional. [1]

M.Sc. (Physics Examination, 2018)

(2^{nd} Year, 1^{st} Semester, Day, 2018)

Condensed Matter Physics - I

Group – B

Answer any two questions

1. (a) For a periodic potential V(x) = V(x+a) define a translation operator Γ such that Γψ (x) = ψ(x+a) and show that [Γ H] = 0.

What is the implication of this commutation relation?
Hence show that amplitude of the wavefunction for an electron incase of the above periodic potential has the same periodicity of the lattice.

(b) The primitive translation vectors of the hexagonal space lattice are given as

$$\vec{a}_1 = \frac{\sqrt{3}}{2}a\,\hat{x} + \frac{a}{2}\hat{y}\,; \quad \vec{a}_2 = -\frac{\sqrt{3}}{2}a\,\hat{x} + \frac{a}{2}\hat{y}\,; \; \vec{a}_3 = c\hat{z}$$

Show that the volume of the primitive cell is $\frac{\sqrt{3}}{2}a^2c$

(ii) show that the primitive translations of the reciprocal lattice are

$$\vec{b}_1 = \left(\frac{2\Pi}{\sqrt{3}}\right)\frac{1}{a}\hat{x} + \frac{2\Pi}{a}\hat{y}\,; \quad \vec{b}_1 = -\left(\frac{2\Pi}{\sqrt{3}}\right)\frac{1}{a}\hat{x} + \frac{2\Pi}{a}\hat{y}\,; \vec{b}_3 = \frac{2\Pi}{c}\hat{z}$$

so that the lattice is its own reciprocal but with a rotation of axes. (You can take the magnification constant 2Π)

Can you draw the Brillouin Zone of the above lattice?

(6+4)

2. (a) Show that the wave functions of a many electron system may be either symmetric or anti-symmetric? Can it be party symmetric or partly antisymmetric?

(b) Show that the determinantal wavefunction satisfy the antisymmetrization rule and also Pauli Principle.

c) What is a symmetric operator? Prove that for a normalized determinantal wavefunction the expectation value of the Hamiltonian of a system of N electrons can be expressed as

$$\langle H \rangle = \sqrt{N!}\int \psi^{*} H \phi_1(x_1)\phi_1(x_2) \ldots\ldots\ldots\ldots\ldots\ldots \phi_N(x_N)\; d\tau'$$

where the symbols have their usual meaning.

(d) Suppose (hkl) are the Miller Indices of a set of planes with respect to $\vec{a}$, $\vec{b}$, $\vec{c}$ the initial unit cell. Find the Miller indices ($h'k'\ l'$) when referred to another set of axes $\vec{a'}\ \vec{b'}\ \vec{c'}$ of the transformed unit cell.

(2 +3 + 3+2)

3 (a) Set up the Hamiltonian for a solid containing N number of atoms, each with z electrons and write down Schrödinger equation. How can you reformulate the Hamiltonian considering the extended nature of the outermost electronic wavefunction and taking the remaining part as ion core.

Show that for free electron system the eigenfunction

$\psi_k\,(\mathrm{r}) = \frac{1}{\sqrt{v}}\, e^{ik.r}$

which is eigenfunction of Hartree equation is also the eigenfunctions of the Hartee-Fock equations.

(b) Suppose from a three dimensional (3D) solid material you made 2D, 1D and 0D materials. Explain how the electronic motion changes with reduction in dimension.

Prove that density of states function is dependent on dimension by the relation

$$D(E)\ \alpha\ E^{\frac{d}{2}-1}$$

Show graphically how the density of state function varies with dimension and explain the variations

(c) Taking Fermi Dirac distribution find an expression for the Fermi level of a 2 dimensional material at absolute zero of temperature.

(4+4+2)

4. Write short notes on (any two)

(i) Geometrical construction of reciprocal lattice

(ii) Coulomb correlation and Fermi hole

(iii) Experimental determination of Density of States

(iv) Schemes for drawing band structures

(5+5)