Ref. No.: Ex/M.Sc./P/II/307/20/2017
Ex/M.Sc./PHY/E/III/307/29/2017

MASTER OF SCIENCE EXAMINATION 2017

2nd Year (day), 1st Semester and 3rd Year (evening), 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) Show that the spatial parts of the wave functions associated with two-electron spin-singlet and spin-triplet states can be expressed in terms of single-electron states, $\{\phi_1(\vec{r}_1), \phi_2(\vec{r}_2)\}$ as

$$\Psi_\pm(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) \pm \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\right].$$

[2]

(b) Let us suppose that the two-electron system is described by the Hamiltonian,

$$H = H_1 + H_2, \quad H_1 = \sum_{i=1}^{2} h_i, \quad h_i = \left(-\frac{\hbar^2}{2m}\nabla_i^2 - \frac{Ze^2}{4\pi\epsilon_0\, r_i}\right), \quad H_2 = \frac{e^2}{4\pi\epsilon_0\, |\vec{r}_1 - \vec{r}_2|},$$

and the single-electron wave functions, $\phi_i(\vec{r}_i)$ satisfy the eigen value equation $h_i\phi_i(\vec{r}_i) = E_i\phi_i(\vec{r}_i)$. Now by treating H_1 as the unperturbed Hamiltonian and H_2 as the perturbation show that singlet and triplet energies are $E_\pm = E_1 + E_2 + I \mp J$, respectively where

$$I = \langle\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)|H_2|\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\rangle \text{ and } J = \langle\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)|H_2|\phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\rangle.$$

[4]

(c) By using the trial wave function of the form

$$\psi(x) = A\, e^{-bx^2},$$

find the bound state energy of a one-dimensional Dirac delta potential, $V(x) = -\alpha\,\delta(x)$.

[4]

2. (a) By using the Hartree-Fock equation,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} + \frac{e^2}{4\pi\epsilon_0}\int \frac{d\vec{r'}}{|\vec{r}-\vec{r'}|}\left(\sum_{j=1}^{N}|\psi_j(\vec{r'})|^2 - \sum_{j=1}^{N\,\prime}\frac{\psi_j^*(\vec{r'})\psi_i(\vec{r'})\psi_j(\vec{r})}{\psi_i(\vec{r})}\right)\right]\psi_i(\vec{r}) = \epsilon_i \psi$$

introduce the exchange charge density at position $\vec{r'}$ for an electron in the ith state at position $\vec{r}$, *i. e.*, $\rho_i^{\mathrm{ex}}(\vec{r},\vec{r'})$. Show that total exchange charge, is

$$\int \rho_i^{\mathrm{ex}}(\vec{r},\vec{r'})\, d\vec{r'} = e,$$

where e is the charge of a proton. [1+1=2]

(b) Estimate the exchange charge density for the electron gas and show that at $T = 0$ K

$$\rho_{\vec{k}}^{\mathrm{ex}}(\vec{r},\vec{r'}) = \frac{ek_{\mathrm{F}}^3}{2\pi^2}\, e^{-i\vec{k}\cdot\vec{R}}\, f(x), \quad f(x) = \frac{1}{4\pi k_{\mathrm{F}}^3}\int e^{i\vec{k}\cdot\vec{R}} d\vec{k} = \frac{\sin x - x\cos x}{x^3}.$$

where $x = k_{\mathrm{F}}R$ and $\vec{R} = \vec{r} - \vec{r'}$. Other symbols have their usual meaning. [2]

(c) Show that the average exchange charge density at position $\vec{r'}$ due to an electron at position $\vec{r}$ for the electron gas is

$$\overline{\rho^{\mathrm{ex}}}(\vec{r},\vec{r'}) = \frac{9\,e\,N}{2\,V}\, f(x)^2.$$

[2]

(d) Thus show that the average charge density at a distance R from an electron at $\vec{r}$ of electrons with parallel spins is

$$-\frac{eN}{2V}\, F(x), \quad \text{where} \quad F(x) = 1 - 9f(x)^2.$$

[2]

(e) Plot the variation of $F(x)$ with x and describe the creation of Fermi hole. [1+1=2]

3. (a) Express the total kinetic energy of N number of non-interacting electrons confined in volume V in terms of number density of electrons (n) by using the Sommerfeld model. Henceforth obtain the expression of Thomas-Fermi kinetic energy functional, $T[n(\vec{r})]$. [2+1=3]

(b) Derive the expression of Hartree potential functional,

$$U[n(\vec{r})] = \frac{e^2}{4\pi\epsilon_0}\,\frac{1}{2}\,\langle\Psi|\sum_j\sum_k \frac{1}{|\vec{r}_j - \vec{r}_k|}|\Psi\rangle$$

by using the expression of electron number density

$$n(\vec{r}) = \sum_j |\psi_j(\vec{r})|^2,$$

where $\psi_j(\vec{r})$s are the normalized single electron wave function and $\Psi(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_N) = \prod_i \psi_i(\vec{r}_i)$. [2]

(c) By using the total energy functional, $E[n] = T[n] + U[n]$, derive the expressions of integral and differential forms of Thomas-Fermi equation. [2]

(d) Solve the Thomas-Fermi equation in the asymptotic region and show that

$$n(\vec{r}) \propto \frac{1}{r^6}, \quad \text{when} \quad r \to \infty.$$

[3]

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]

Ex/M.Sc./Phy/III/I/307/29/2017

Ex/M.Sc./Phy/II/307/20/2017

M.Sc. (Physics Examination, 2017

(2nd Year, 1st Semester, 2017)

(3rd Year 1st, Semester, Evening)

Condensed Matter Physics - I

Group - B

Answer any two questions

1. (a) Define density of state function.

Show that the density of state function depends upon dimension 'd' of the solid by the following relation

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

(b) Plot graphically the variation of Density of state functions for (i) Two dimensional solid, (ii) One dimensional solid and (iii) Zero dimensional solid; Explain the physical significance of such plots.

(c) Obtain an expression for the Fermi level of a 2 dimensional solid at absolute zero considering its density of state function.

(5 + 3 + 2)

2 (a) For a one dimensional potential explain the following schemes for drawing E-K diagrams in a solid

(i) Periodic zone scheme
(ii) Reduced zone scheme
(iii) Extended zone scheme

Show the first and second Brillouin zone for the above schemes. What is Wigner-Seitz cell?

(b) Construct the first four Brillouin Zones for a simple cubic lattice in two dimensions.

(c) By assuming a flat emitting surface and applying the concept of image charge show that the reduced barrier with the application of an external field can be expresses as

$$V = -e\sqrt{eE}$$ where the symbols have their usual meanings.

Hence explain the Schottkey effect.

(3+ 3 + 4)

3. (a) Derive the following expression for susceptibility of Pauli paramagnetism formula for a metal

$$\chi_p = \frac{3\,n\,\mu_B^2}{2\,k_B T_F}$$

where the symbols have their usual meanings.

Does the result tally with experiment? If not explain why?

(b) Write down Boltzmann Transport equation and explain the different terms in it. Solve this equation for finding an expression for the current density in a metal under relaxation time approximation.

(5 + 5)