MASTER OF SCIENCE EXAMINATION, 2024

(2nd Year, 1st Semester)

PHYSICS

PAPER : PHY/TE/307

(Condensed Matter Physics - I)

Time : *Two Hours* *Full Marks* : 40

(20 marks for each group)

Use separate Answer Script for each group.

GROUP—A

Answer ***any two*** questions.

1. *(a)* Show that eigenvalues of two-particle exchange operator, $\mathcal{P}$, for the many-particle quantum states of identical and indistinguishable particles are ± 1.

   (b) Let us suppose that $\{\phi_{\nu}(r)\}$ forms a complete orthonormal set of single-particle basis states and consider that $V_{jk} = V(r_j - r_k)$ is a two-particle operator. Show that sum of V_{jk}, *i.e.*, $V = \frac{1}{2}\Sigma_{jk} V_{jk}$, for a N-particle system satisfies the relation,

$$V \,|\, \phi_{\nu_{n_1}}(r_1) | \cdots \phi_{\nu_{n_N}}(r_N) \rangle = \frac{1}{2} \sum_{jk;\, \nu_c \nu_d \nu_a \nu_b} V_{\nu_c \nu_d,\, \nu_a \nu_b} \delta_{\nu_a \nu_{n_j}}, \delta_{\nu_b \nu_{n_k}} |\, \phi_{\nu_{n_1}}(r_1)$$

$$\cdots \phi_{\nu_c}(r_j) \cdots \phi_{\nu_d}(r_k) \cdots \phi_{\nu_{n_N}}(r_N) |,$$

where $V_{v_c v_d, v_a v_b} = \langle \phi_{v_c}(r_j)\,\phi_{v_d}(r_k) | V_{jk} | \phi_{v_a}(r_j)\phi_{v_b}(r_k) \rangle$.

(c) Show that in the second quantization representation, V could be expressed as

$$V = \frac{1}{2} \sum_{v_i v_j v_k v_l} V_{v_i v_j, v_k v_l}\, c^{\dagger}_{v_i} c^{\dagger}_{v_j} c_{v_l} c_{v_k},$$

where c is the fermionic annihilation operator.

(d) Now considering the free-particle states as the single-particle basis states, where

$$V_{v_i v_j, v_k v_l} = \sum_{\sigma\sigma'} \int\!\!\int dr\, dr'\, \phi^{*}_{v_i\sigma}(r)\, \phi^{*}_{v_j\sigma'}(r') \frac{e^2}{4\pi\varepsilon_0 |r - r'|} \phi_{v_k\sigma}(r)\, \phi_{v_l\sigma'}(r'),$$

and $\phi_{v\sigma}(r) = \dfrac{1}{\sqrt{V_0}} e^{i k\cdot r} \chi_\sigma$, show that by using

$$\int dr\, \frac{e^{i\, q\cdot r}}{r} = \frac{4\pi}{q^2},$$

$$V = \frac{e^2}{\varepsilon_0 V_0} \sum_{\sigma\sigma'} \sum_{k_1 k_2 q} \frac{1}{q^2}\, c^{\dagger}_{k_1+q\sigma}\, c^{\dagger}_{k_2-q\sigma'}\, c_{k_2\sigma'}\, c_{k_1\sigma}.$$

[1+2+2+5=10]

2. *(a)* In the second-quantization theory consider the many-particle Hamiltonian for two kinds of particles, (a and b) as,

$$H = H_0 + V,$$

(c) Write the various ways of solving the above equation. Find a solution of the above equation under relaxation time approximation. (2+6+2)=10

4. Write short notes (***any two***) : (5+5)=10

(a) Geometrical construction of reciprocal lattice

(b) Dimensional dependence of electrical and optical properties of solids

(c) Different schemes of drawing band structure

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

(b) Find the matrix of transformation for the indices between the conventional hexagonal unit cell and the alternative orthorhombic unit cell. Draw the necessary diagram.

(c) Considering a set of $(h\,k\,l)$ planes elucidate the Ewald's construction. Show that Bragg condition is satisfied when the reciprocal lattice point of such planes lie on the sphere. What happens when the crystal is rotated? Explain the significance of such construction.

(4+2+4)=10

3. *(a)* What are the limitations of Drift-diffusion model of carrier transport in a solid?

(b) Defining a carrier distribution function $f(\vec{r}, \vec{k}, t)$ obtain the following relation

$$\frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} + \vec{v}(\vec{k}).\nabla_r\, f(\vec{r}, \vec{k}, t) + \frac{\vec{F}(\vec{r}, t)}{\hbar}.\nabla_k\, f(\vec{r}, \vec{k}, t)$$
$$= \sum_{k'} S(\vec{k'}, \vec{k})\, f(\vec{r}, \vec{k}, t)[1 - f(\vec{r}, \vec{k}, t)]$$
$$- \sum_{k'} S(\vec{k}, \vec{k'})\, f(\vec{r}, \vec{k}, t)[1 - f(\vec{r}, \vec{k'}, t)]$$

where the symbols have their usual meanings. Explain the physical meaning of the different terms.

where

$$\begin{cases} H_0 = \sum_\nu t_\nu^a\, a_\nu^\dagger\, a_\nu + \sum_\mu t_\mu^b\, b_\mu^\dagger\, b_\mu, \\ V = \sum_{\nu\nu'\mu\mu'} V_{\nu\mu\nu'\mu'}\, a_\nu^\dagger\, b_\mu^\dagger\, b'_\mu\, a'_\nu. \end{cases}$$

By assuming the interaction between different kind of particle is important *(i)* develop the Mean-field theory and *(ii)* show that the expressions of one Mean-field parameter

$$\langle a_\nu^\dagger\, a_\nu \rangle = \frac{1}{Z_{\mathrm{MF}}} \mathrm{Tr}(e^{-\beta H_{\mathrm{MF}}} a_\nu^\dagger\, a_\nu)\ .$$

(iii) Obtain the total Mean-field Hamiltonian.

(b) Consider the total electron-electron Coulomb interaction potential as,

$$V = \frac{1}{2} \sum_{\nu\nu'\mu\mu'} V_{\nu\mu\nu'\mu'}\, c_\nu^\dagger\, c_\mu^\dagger\, c'_\mu\, c'_\nu\ .$$

Show that after Hartree-Fock approximation the total potential can be written as

$$V_{HF} = \sum_{\nu\mu} [V_{\nu\mu\nu\mu} - V_{\nu\mu\mu\nu}]\, c_\nu^\dagger\, c_\nu\, \bar{n}_\mu + \text{Constant}.$$

(c) Now considering the interacting electrons are confined within a box of volume ν and the single particle wave functions are

$$\psi_{k,\sigma} = \frac{1}{\sqrt{\nu}} e^{ik\cdot r} \chi_\sigma\ ,$$

show that the Fock energy of an electron is

$$V_{k\sigma}^F = \frac{e^2}{\varepsilon_0 \nu} \sum_{k'} \frac{n_{k'\sigma}}{|k' - k|^2}\ .$$

Symbols have their usual meanings.[(2+1+1)+3+3=10]

3. Consider the formulation of valence-bond (Hitler-London) theory on the hydrogen molecule (H_2), where the relevant Hamiltonian is

$$\mathcal{H}(r_1, r_2) = \mathcal{H}_A(r_1) + \mathcal{H}_B(r_2) + \mathcal{H}_{\text{int}}(r_1, r_2),$$

and

$$\begin{cases} \mathcal{H}_A(r_1) = -\dfrac{h^2}{2m}\nabla_1^2 - \dfrac{e_0^2}{|r_1 - r_A|} \\ \mathcal{H}_B(r_2) = -\dfrac{h^2}{2m}\nabla_2^2 - \dfrac{e_0^2}{|r_2 - r_B|}, \\ \mathcal{H}_{\text{int}}(r_1, r_2) = \dfrac{e_0^2}{|r_1 - r_2|} + \dfrac{e_0^2}{|r_A - r_B|} - \dfrac{e_0^2}{|r_1 - r_B|} - \dfrac{e_0^2}{|r_2 - r_A|}, \\ e_0^2 = \dfrac{e^2}{4\pi\varepsilon_0}. \end{cases}$$

Symbols have their usual meanings.

(a) Construct the total antisymmetric wave functions in terms of spin singlet and spin triplet states as

$$\Psi(r_1, \sigma_1, r_2, \sigma_2) = \begin{cases} \psi_s(r_1, r_2)\,\chi_s(\sigma_1, \sigma_2), \\ \psi_t(r_1, r_2)\,\chi_t(\sigma_1, \sigma_2), \end{cases}$$

and write the expressions of $\psi_s(r_1, r_2)$, $\psi_t(r_1, r_2)$, $\chi_s(\sigma_1, \sigma_2)$, and $\chi_t(\sigma_1, \sigma_2)$.

(b) Show that the normalization constants for the symmetric/antisymmetric spatial wave functions can be written as

$$N_{\pm} = \frac{1}{\sqrt{2(1 \pm |\mathcal{S}_{AB}|^2)}},$$

where the symbols have their conventional meanings.

(c) Show that the energies of the singlet/triplet states are respectively,

$$E_{s/t} = 2E_0 + 2N_{\pm}^2(C \pm J).$$

The symbols have their conventional meanings.

[3+3+4=10]

GROUP—B

*Answer **any two** questions.*

1. (a) Define periodic boundary conditions.

Considering a three-dimensional potential box with potential defined as $V(r) = 0$ inside the box and ∞ otherwise and with the help of periodic boundary condition show that density of state can be expressed as $D(E) = \dfrac{1}{4\pi^2}\left(\dfrac{2m}{\hbar^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}}$

Show that the density of state function depends upon dimension d of the solid by the following relation $D(E) \propto E^{\frac{d}{2}-1}$

(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 and one-dimensional solid at absolute zero considering its density of state function.

(d) Discuss an experimental method to determine the density of state of a solid. (4+3+1½+1½)=10