(c) What is electronic specific heat of a metal? Show that the electronic specific heats of a metal at very low temperature can be represented as

$$C_{el} = \frac{1}{3}\pi^2 N K_B \frac{T}{T_F}$$

where the symbols have their usual meanings.

How can you separate lattice specific and electronic specific heat from the measured specific heat of a metal? 3+3+4

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Ex/SC/PHY/PG/CBS/TH/208/2025

M. Sc. Examination, 2025

[2nd Year 1st Semester (Day)]

PHYSICS

Paper : PHY/TH/208

(Condensed Matter Physics – I)

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

(**20** marks for each Group)
Use separate answer scripts for each Group.

Group—A

Answer *any* **two** questions : 10×2=20

1. **(CO1, CO2)** *(a)* Let us suppose that $\{\phi_v(r)\}$ forms a complete orthonormal set of single-particle basis states and $T = \sum_{j=1}^{N} T_j$, a sum of one-particle operator, T_j. Show that T satisfies the relation,

$$T\left|\phi_{v_{n_1}}(r_1)\cdots\phi_{v_{n_N}}(r_N)\right\rangle = \sum_j \sum_{v_a v_b} T_{v_b v_a}\delta_{v_a, v_{n_j}}\left|\phi_{v_{n_1}}(r_1)\cdots\phi_{v_b}(r_j)\cdots\phi_{v_{n_N}}(r_N)\right\rangle,$$

Where $T_{v_b v_a} = \left\langle \phi_{v_b}(r_j)\middle|T_j\middle|\phi_{v_a}(r_j)\right\rangle$.

(b) Show that in the second quantization representation, T could be expressed as

$$T = \sum_{v_a v_b} T_{v_a v_b} C^\dagger_{v_a} C_{v_b}$$

(c) By using the single-particle momentum operator, $p = -i\hbar\nabla$, in first quantization, obtain the second quantized many-particle momentum operator in the momentum eigenket basis states, i.e., $p = \sum_k hk\, a^\dagger_k a_k$.

(d) Show that the second quantized form of density operator $\rho(r) = \delta(r - r')$ in momentum eigenket representation is

$$\rho(r) = \frac{1}{V_0}\sum_q \left(\sum_k c^\dagger_k c_{k+q}\right) e^{iq\cdot r} = \frac{1}{V_0}\sum_q \rho(q) e^{iq\cdot r},$$

where $\rho(q) = \sum_k c^\dagger_k c_{k+q}$ is the Fourier component of $\rho(r)$. 3+3+2+2=10

2. (CO3) Consider the SSH model,

$$H_{SSH} = \sum_n \left[t(a^\dagger_n b_n + b^\dagger_n a_n) + t'(b^\dagger_n a_{n+1} + a^\dagger_{n+1} b_n) \right]$$

(a) Express the Hamiltonian in the momentum space by using the Fourier transform of the operators as

$$a_n = \frac{1}{\sqrt{N}} \sum_k e^{ik\cdot R_n} a_k,$$

$$b_n = \frac{1}{\sqrt{N}} \sum_k e^{ik\cdot R_n} b_k.$$

(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) For diffraction of X-rays from a set of crystal planes if $\vec{k}$ is the wave vector of the incident wave and $\vec{k'}$ is that of the reflected wave and $\vec{g}$ is the reciprocal lattice vector, then prove the following relation: $2\vec{k}.\vec{g} + g^2 = 0$. 4+2+4

2. (a) Show that density of state function of a crystalline solid in 2D is independent of energy.

(b) Explain qualitatively the variation of density of states of 2D and 1D solids with energy clearly explaining the nature of plots.

How can you experimentally verify the above types of density of states?

(c) Consider a triangular lattice in two dimensions. Find the first Brillouin zone. Given an arbitrary wavevector k (in two dimensions), write an expression for an equivalent wavevector within the first Brillouin zone. 3+5+2

3. (a) Clearly explain the geometrical construction of reciprocal lattice. What are the advantages of going to reciprocal space?

(b) Show that the volume of the first Brillouin zone is $\frac{(2\pi)^3}{V_c}$; where V_c is the volume of crystal primitive cell.

(b) Obtain the expressions of *(i)* eigenvalues and *(ii)* eigenvectors.

(c) Show that the expression of Pancharatnam-Berry phase of one eigenvector is

$$\gamma = \frac{1}{2}\oint \frac{t'^2 + tt'\cos k}{t^2 + t'^2 + 2tt'\cos k}\, dk.$$

3+(2+2)+3=10

3. **(CO4)** 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

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

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

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

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

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