QCMP-2020/21 **Quantum Condensed Matter Physics**

Problem sheet 4: **Semiconductor devices, interacting electron systems**

1. **Depletion layer**

   A full treatment of this problem requires the solution of the Poisson equation to determine the electric field distribution $V(x)$ combined with the thermal carrier statistics to determine the occupancy of the states. At low temperature, when the boundary of the depletion regime may be assumed to be sharp, it is more straightforward.

   A metal-semiconductor contact is made between a perfect conductor and a uniformly doped n-type semiconductor with a donor density N_d. Assume that the temperature is low enough that the donor levels are completely filled or completely empty. By solving Poisson's equation, show that in the depletion region $0 < x < x_b$ the potential satisfies

   $$\phi = \phi_b - \frac{N_d e}{2\epsilon\epsilon_0}(x_b - x)^2 \tag{1}$$

   Estimate the depletion width for a semiconductor with $\epsilon = 12$, $e\phi_b = 0.5\ eV$, and $N_d = 10^{22}\ m^{-3}$.

2. **Quantum well sub-bands**

   A 10 nm thick quantum well of GaAs is surrounded by bulk $Al_{0.7}Ga_{0.3}As$. The conduction band offset is 0.26 eV, and the effective mass of electrons in GaAs is 0.066 m_e.

   (a) Estimate the energies of the (bottom of the) sub-bands $E_n(\mathbf{k} = 0)$, assuming the walls of the potential are infinitely high.

   (b) What is the maximum areal density of electrons that can be occupied in the lowest sub-band before the second sub-band starts to be filled?

   (c) How many sub-bands do you estimate exist for the actual sitation — a well of finite potential depth?

   (d)* *Note the word* **estimate** *in (c). Nevertheless, the 1D finite potential well is not a difficult problem to solve, though the actual solution of eigenstate energies needs to be done graphically.*

   For a potential of depth V_0 and width L, show that the number of bound states is

   $$1 + \text{Int}\left[(2m^*V_0L^2/\pi^2\hbar^2)^{1/2}\right]. \tag{2}$$

3. **Brief notes 1**
   Write brief notes about

   - $p - n$ junctions and the $p - n$ junction diode $I - V$ characteristic.
   - Light emitting diodes and solar cells.
   - Field effect transistors.

4. **Peierls transition**

   Consider a one-dimensional system which is filled up to the first Brillouin zone boundary at $k = \pi/a$, and assume that there is a small gap produced by a single Fourier component of

the lattice potential $U = U_{K=2\pi/a}$ (small meaning that $U/E^0_{\frac{1}{2}K} \ll 1$). Consider momenta close to the zone boundary, and show that a good approximation for the energy dispersion of the bands is

$$E = E_0 \left(1 \pm \sqrt{\frac{U^2}{E_0^2} + 4\kappa^2} \right)$$

where $E_0 = E^0_{\frac{1}{2}K}$ and $k = (\pi/a)(1 + \kappa)$, with $\kappa \ll 1$.

(*) Show that the change in electronic energy

$$E_{elec} = \frac{1}{N} \sum_{k \ occupied} [E(k; U_K) - E(k; U_K = 0)]$$

can be written approximately as

$$E_{elec} = |U| \int_0^1 dx \left[\frac{x}{\alpha} - (1 + \frac{x^2}{\alpha^2})^{1/2} \right] \propto \frac{\hbar^2 \pi^2}{ma^2} \alpha^2 \log(\alpha) \ ,$$

in the limit that the parameter $\alpha = \frac{ma^2}{\hbar^2\pi^2}|U|$ is much smaller than unity (i.e. the gap is small compared to the bandwidth.)

5. **Covalent bonds are singlets**

   How is it that electrons in a covalent bond - e.g. H_2 - are almost invariably in singlet states? The two atomic states that make up the wavefunction are not orthogonal, and so the charge density is not independent of the spin-state of the ions. The singlet state will lead to a charge density that is more favourable for strong bonds than the triplet.
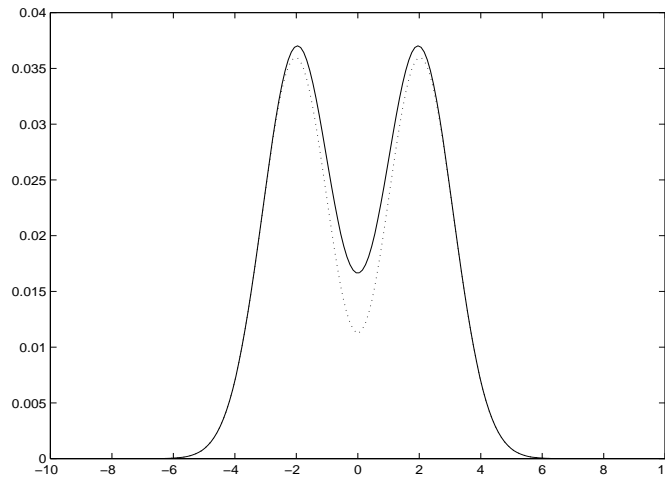

Figure 1: A sketch of the charge density for the wavefunctions in a singlet state (solid line) and a triplet state(dotted line) for two overlapping gaussian orbitals in (3)

Consider single-particle wavefunctions on two neighbouring identical atoms ψ_A, ψ_B, which may be assumed real. These are to be used as the basis for a two-electron state. Show that the charge density in a singlet (triplet) state made out of the two orbitals is given by

$$\rho(r) = |\psi_A(r)|^2 + |\psi_B(r)|^2 \pm 2 < \psi_A|\psi_B > \psi_A(r)\psi_B(r) \quad . \tag{3}$$

By reference to Fig. 1, explain why the singlet state will usually be lower in energy.

6. **Curie law**
   An exercise in statistical physics that you may well have seen before.

   Using

   $$M = -\frac{1}{V}\frac{\partial F}{\partial H}, \tag{4}$$

   and the partition function

   $$Z = e^{-\beta F} = \sum_{J_z=-J}^{J} e^{-\beta g_L \mu_B H J_z} \quad \beta = 1/k_B T\ , \tag{5}$$

   derive the Curie law and the conditions for its validity.

7. **Brief notes 2**

   - Show how the spin-independent Coulomb repulsion between electrons can give rise to a spin-dependent exchange interaction.

   - State the line of argument underlying Fermi liquid theory.

   - List the key phenomena associated with heavy fermion materials and discuss their interpretation in terms of massive quasiparticles.

   - Explain how ferromagnetism in metals can be explained from Stoner's band model.

   - Explain the formation of charge density wave order via a Peierls transition.

8. **Band magnets**
   The three metals calcium (Ca), scandium (Sc) and palladium (Pd) have experimentally observed susceptibilities χ significantly higher than the Pauli susceptibilities χ_P calculated from their densities of states $g(E_F)$ (as obtained, for example, from specific heat capacity measurements at low temperature):

Metal	χ/χ_P	$g(E_F)$ (eV^{-1})
Ca	4.5	1.8
Sc	6.1	2.5
Pd	4.5	2.4

   Table 1: Susceptibility enhancement χ/χ_P and density of states at the Fermi level $g(E_F)$ for three metals

   (a) State Stoner's expression for the exchange-enhanced susceptibility of a metal and explain the origin of the observed enhancement in Ca, Sc and Pd.

   (b) Use the values from the table to extract the Stoner parameter (or Coulomb repulsion, or exchange and correlation energy) U for each metal.

   (c) Iron, cobalt and nickel have Stoner parameters $U \simeq 0.5$ eV. Put a lower bound on the Sommerfeld coefficients ($\gamma = C_m/T$) of these three metals.

9. **Antiferromagnet in mean field approximation**
   An antiferromagnetic insulator consists of two sub-lattices. The magnetisation of the first sublattice is M_1, the magnetisation of the second sublattice is M_2. We want to arrive at the ordering temperature and $M_{1,2}(T)$ curves of this material by considering a mean

field model. To achieve this, we write the equations of state ($M - H$ curves) of the two sublattices as:

$$a_1(T)M_1 + b_1 M_1^3 = H + \lambda_1 M_2 \tag{6}$$
$$a_2(T)M_2 + b_2 M_2^3 = H + \lambda_2 M_1 \tag{7}$$
$$\tag{8}$$

(a) Explain the meaning of the symbols in these equations and state the temperature dependence of a_1 and a_2.

(b) At zero applied field we can set $H = 0$ and solve the two coupled equations. If we want to focus only on the region near the ordering temperature T_N, then it is useful to approximate from the second equation:

$$M_2 \simeq \frac{\lambda_2}{a_2} M_1$$

and substitute this into the first equation for M_2 (and likewise for the second equation). Find the resulting decoupled equations for M_1 and M_2.

(c) Inserting the temperature dependences of $a_1(T)$ and $a_2(T)$, extract the ordering temperature T_N and the temperature dependence of the sublattice magnetisation $M_1(T), M_2(T)$ close to T_N.

Note: Starred questions are challenge problems; they will do you good, but they go beyond the minimum requirements of the course.