QCMP-2014/15 — Quantum Condensed Matter Physics

Problem sheet 1: Lorentz dipole oscillator model, Drude model, Sommerfeld theory, lattices

1. **Sapphire**
   A sapphire crystal doped with titanium absorbs strongly around 500 nm. Calculate the difference in the refractive index of the doped crystal above and below the 500 nm absorption band, if the density of absorbing atoms is $1 \cdot 10^{25}$ m^{-3}. The refractive index of undoped sapphire is 1.77.

2. **Reflectivity of metals**

   The phase velocity of light in a conducting medium is the speed of light divided by the refractive index $N(\omega) = \epsilon(\omega)^{1/2}$ where we may use for ϵ the Drude result

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega/\tau} \quad . \tag{1}$$

   In a "good" metal, we have $1/\tau \ll \omega_p$.

   Show that

   (a) For $\omega \ll 1/\tau$, ϵ is large and imaginary, so that $|N| \gg 1$ and N has roughly equal real and imaginary parts,

   (b) For $1/\tau \ll \omega \ll \omega_p$, ϵ is real and negative, so that N is imaginary,

   (c) For $\omega > \omega_p$, ϵ is positive, and N is real.

   Consider a light wave with the electric field polarised in the $x-$direction at normal incidence from the vacuum on a good Drude metal (with $1/\tau \ll \omega_p$) occupying the region $z > 0$. In the vacuum ($z < 0$), the incident E_1 and reflected E_2 waves give rise to a field

$$E_x = E_1 \exp(i\omega[z/c - t]) + E_2 \exp(-i\omega[z/c + t]) \quad , \tag{2}$$

   whereas in the medium, the electric field is

$$E_x = E_0 \exp(i\omega[N(\omega)z/c - t]) \quad . \tag{3}$$

   Matching the electric and magnetic fields on the boundary, show that

$$\begin{aligned} E_0 &= E_1 + E_2 \quad , & (4) \\ NE_0 &= E_1 - E_2 \quad , & (5) \end{aligned}$$

   and hence show that the reflection coefficient satisfies

$$R = \left|\frac{E_2}{E_1}\right|^2 = \left|\frac{1-N}{1+N}\right|^2 \quad . \tag{6}$$

   Using the Drude formula above, show that

$$\begin{aligned} R &\approx 1 - 2\left(\frac{2\epsilon_0\omega}{\sigma(0)}\right)^{1/2} \quad \text{for } \omega \ll 1/\tau & (7) \\ &\approx 1 - \frac{2}{\omega_p\tau} \quad \text{for } 1/\tau \ll \omega \ll \omega_p & (8) \\ &\approx \frac{1}{16}\left(\frac{\omega_p}{\omega}\right)^4 \quad \text{for } \omega_p \ll \omega & (9) \end{aligned}$$

and sketch the reflectivity $R(\omega)$.

To get the first two of these results with the minimum of fuss, you may find it helpful to expand in $1/N$, viz.

$$R = \frac{(1-\frac{1}{N})(1-\frac{1}{N^*})}{(1+\frac{1}{N})(1+\frac{1}{N^*})} \approx 1 - 4\Re(1/N) \tag{10}$$

3. **Optical properties of solids**

Discuss why, at optical frequencies, glass is transparent, and silver is shiny, while graphite appears black, and powdered sugar is white.

4. **Static conductivity tensor**

Show that in the presence of a magnetic field $\mathbf{B}$ aligned along the z-axis, the electrical conductivity can be written as a tensor $\mathbf{j} = \sigma \cdot \mathbf{E}$, with

$$\sigma = \frac{\sigma_o}{1+\beta^2} \begin{pmatrix} 1 & \beta & 0 \\ -\beta & 1 & 0 \\ 0 & 0 & 1+\beta^2 \end{pmatrix} \tag{11}$$

Here $\omega_c = \frac{qB}{m^*}$, $\beta = \omega_c \tau$ and $\sigma_o = ne^2\tau/m^*$. The carrier charge q can be $+e$ or $-e$.

In a high magnetic field ($\beta \gg 1$), show that $\sigma_{xy} = -\sigma_{yx} = nq/B$.

5. **Density of states for free electrons**

(a) What is the Fermi wavevector and Fermi energy as a function of particle density for a free electron gas in one and two dimensions (define density appropriately)?

(b) Calculate the density of states in energy for free electrons in one and two dimensions. [Answer:$(2m/\pi\hbar^2) \times (\hbar^2/2mE)^{\frac{1}{2}}$, (d=1); $(m/\pi\hbar^2)$, d=2; $(m/\pi^2\hbar^2) \times (2mE/\hbar^2)^{\frac{1}{2}}$, d=3 .]

(c) Show how the 3D density of states can be re-written as

$$(3/2)(n/E_F)(E/E_F)^{\frac{1}{2}}$$

with $n = N/V$.

6. **Thomas-Fermi screening**

Show that in a metal, a spatially modulated external potential with wavenumber q and amplitude $V_{ext}(q)$, induces a spatially oscillating number density n_{ind} with amplitude

$$n_{ind}(q) = \frac{\epsilon_0 q^2}{e} \frac{V_{ext}(q)}{\left[1 + q^2/q_{TF}^2\right]} ,$$

with $q_{TF}^2 = \frac{1}{\pi^2}\frac{me^2}{\epsilon_0\hbar^2}k_F = \frac{4}{\pi}\frac{k_F}{a_B} = (\frac{2.95}{\sqrt{r_s}}\text{Å}^{-1})^2$, the Thomas-Fermi wavevector.

For the potential generated by a localised impurity of charge Q, $V_{ext} = Q/(4\pi\epsilon_0 r)$, show that the induced charge density is then of the form

$$n_{ind}(r) \propto \frac{e^{-r/\xi}}{r}$$

and identify the screening length ξ.

7. **Diatomic molecule**

This is a simple problem to illustrate the physics of a diatomic molecule. It also provides an elementary example of the *Linear Combination of Atomic Orbitals* (LCAO), or tight binding method, which we shall be using later to describe extended solids.

We restrict the basis of states to just the ground state of each atom in isolation, whereas of course an accurate solution would require a complete set of states that of necessity would include all the excited states of the atoms. The basis set consists of two states $|a>$ and $|b>$ that satisfy

$$H_a|a> \;=\; E_a|a> \tag{12}$$
$$H_b|b> \;=\; E_b|b> \tag{13}$$

and we look for solutions

$$|\psi>= \alpha|a> + \beta|b> \tag{14}$$

Neglecting the direct matrix elements $< a|b >$ for simplicity (these are easily included if necessary), derive the matrix equation for the wavefunctions and eigenvalues

$$\begin{pmatrix} H_{aa} - E & H_{ab} \\ H_{ba} & H_{bb} - E \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0 \tag{15}$$

where the matrix elements are of two kinds:
Onsite, or *crystal field* terms

$$H_{aa} = \langle a\,|T + V_a + V_b|\,a\rangle = E_a + \langle a\,|V_b|\,a\rangle = \tilde{E}_a \tag{16}$$

Offsite, or *hopping* terms

$$H_{ab} = \langle a\,|T + V_a + V_b|\,b\rangle = t \tag{17}$$

(Note that the sign of t depends on the symmetry of the orbitals: for s-states, with an attractive potential $V_i < 0$, then t is negative; but for p_x states t is positive for atoms aligned along x.)

Solve for the wavefunctions and eigenvalues, for $t < 0$.

Sketch the wavefunctions and charge densities for the lower and upper states, in the cases of (a) identical atoms $\tilde{E}_a = \tilde{E}_b$, and (b) the strongly ionic limit $\tilde{E}_a - \tilde{E}_b \gg |t|$

8. **BCC and FCC lattices**
Show that the reciprocal lattice of a body centred cubic lattice (BCC) of spacing a is a face centred cubic (FCC) lattice of spacing $4\pi/a$; and that the reciprocal lattice of a FCC lattice of spacing a is a BCC lattice of spacing $4\pi/a$.

9. **Reciprocal lattice cell volume**
Show that the volume of the primitive unit cell of the reciprocal lattice is $(2\pi)^3/\Omega_{cell}$, where Ω_{cell} is the volume of the primitive unit cell of the crystal.

10. **Bragg's law**
(a) Show that the reciprocal lattice vector $\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_2$ is perpendicular to the (hkl) plane of the crystal lattice.
(b) Show that the distance between two adjacent (hkl) planes is $2\pi/|\mathbf{G}|$.
(c) Show that the condition $\mathbf{k} \cdot \frac{\mathbf{G}}{2} = (\frac{G}{2})^2$ may be written as

$$\frac{2\pi}{\lambda} \sin\theta = \frac{\pi}{d} \tag{18}$$

where $\lambda = 2\pi/k$, and θ is the angle between the incident beam and the crystal plane.

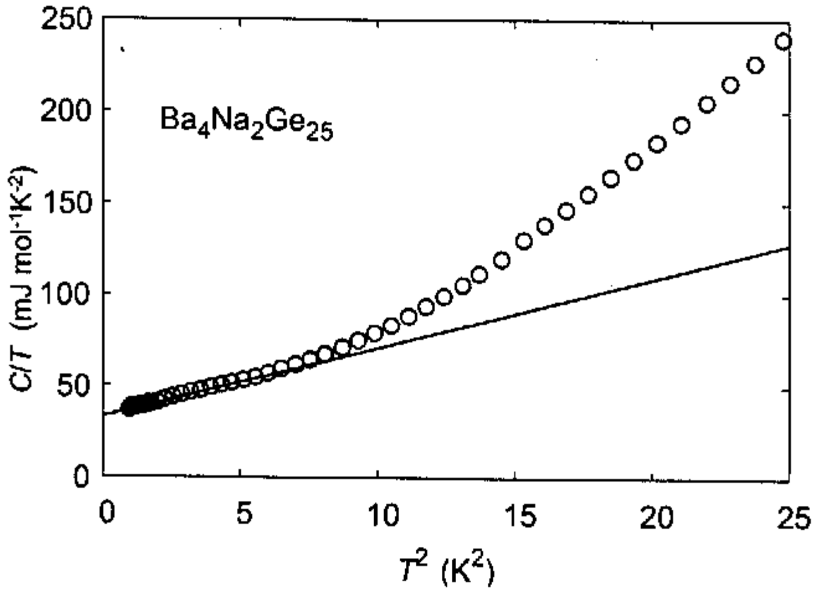
11. **Acoustic phonon dispersion in the monatomic chain**
The equation of motion for a chain of atoms of mass m, which are coupled together by springs with spring constant K, is $m\ddot{u}_n = K(u_{n+1} - u_n) + K(u_{n-1} - u_n)$. Use a plane wave trial function for the displacement of atom n, $u_n(t) = u_o cos(qr_n - \omega(q)t)$, to derive the dispersion relation for the one-dimensional monatomic chain:

$$m\omega^2(q) = 2K(1 - \cos(qa)) = 4K\sin^2(\frac{qa}{2})$$

12. **Heat capacity of a metal**
Show that the molar heat capacity C of metals at low temperature, T, takes the form

$$C = \gamma T + \beta T^3 \quad ,$$

where $\gamma = \frac{\pi^2}{3}k_B^2 g(E_F)$ and $\beta = \frac{12\pi^4}{5}N_A k_B \theta_D^{-3}$ are material dependent constants. $g(E_F)$ is the molar density of states at the Fermi energy, E_F, θ_D is the Debye temperature and N_A is Avogadro's number. [*It is not necessary to deduce the precise form of the numerical prefactors.*]



The graph above shows the heat capacity per mole of the metallic compound $Ba_4Na_2Ge_{25}$, measured to 5 K and plotted as C/T vs. T^2. The line is a linear fit to the low-temperature region. The molar volume of $Ba_4Na_2Ge_{25}$ is $V_m = 4.6 \cdot 10^{-4}$ m^3.

From the measured data, extract the parameter γ and find $g(E_F)$. Assuming a free electron model with a single, parabolic band and two conduction electrons per formula unit, estimate the Fermi energy and the Fermi wavevector, k_F. Would you expect the Fermi wavevector computed above to lie inside or outside the first Brillouin zone?

From the measured data, extract the parameter β and find θ_D. Estimate the Debye wavevector k_D and the speed of sound in this material.

Why does the measured heat capacity at temperatures $T^2 > 10$ K^2 deviate significantly from the low temperature form discussed above? What form do you expect the molar heat capacity to take at even higher temperatures $T >> \theta_D$?

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