Solutions Exam 2015

1 a)

E_1 = macroscopic depolarisation field. Relates to the sample shape and the far field net polarisation of the whole sample.

E_2 = Lorentz-field. A virtual field correcting for the effect of surface polarisation on a cut-out sphere used to calculate the microscopic near-field contributions at the central lattice point coincident with the origin of the sphere. The Lorentz field is mesoscopic.

E_3 = A sum of the microscopic field contributions from all dipoles inside the cut-out sphere as they apply to the lattice point at the sphere origin.

All atoms in lattice points w. cubic symm, $x_i = y_i = z_i$; dipole contribution p(+/-) per atom, E_3 at the central lattice point at the origin:

$$\vec{E}_3 = \sum_{\substack{inside \\ sphere}} \vec{E}_{dipole} = \sum_{\substack{inside \\ sphere}} \frac{3(\vec{p}_i \cdot \vec{r}_i) \cdot \vec{r}_i - r_i^2 \vec{p}_i}{4\pi\varepsilon_0 r_i^5}$$

$$= \frac{p_+}{4\pi\varepsilon_0} \sum_{\substack{+ions \\ inside \\ sphere}} \frac{2z_i^2 - x_i^2 - y_i^2}{r_i^5} + \frac{p_-}{4\pi\varepsilon_0} \sum_{\substack{-ions \\ inside \\ sphere}} \frac{2z_i^2 - x_i^2 - y_i^2}{r_i^5} = 0 + 0$$

1 b) The Maxwell relations in the absence of external fields (no free charges, no magnetisation)

$\quad$ i. $\nabla \times \vec{E} = (\vec{k} \times \vec{E}_0)e^{i\vec{k}\cdot\vec{r}} = 0 \implies \vec{E} = 0 \quad$ or $\quad \vec{E}_0 \parallel \vec{k}$

$\quad$ ii. $\nabla \cdot \vec{D} = \vec{k} \cdot \vec{D}_0 e^{i\vec{k}\cdot\vec{r}} = 0 \implies \vec{D} = 0 \quad$ or $\quad \vec{D}_0 \perp \vec{k}$

$\quad$ Case i:

$$\vec{P} \parallel \vec{k} \text{ :) longitudinal mode.} \quad \varepsilon(k) = 0 \Rightarrow \vec{D} = 0 \Rightarrow \vec{E} = \frac{-\vec{P}}{\varepsilon_0}$$

$\quad$ Case ii: $\quad \vec{P} \perp \vec{k}$:) transversal mode.

$$\vec{E} = 0 \Rightarrow \varepsilon(k) = \frac{\vec{D}}{\varepsilon_0 \vec{E}} \to \infty \Rightarrow \varepsilon(k, \omega = 0) \to \infty$$

The non-zero dielectric response function relates to transversal modes. The result indicates that spontaneous polarisation will occur for all values of k, but may only be valid in the long-λ limit. We must restrict ourselves to long λ, since the polarisation, and hence the dielectric response function, must be expected to vary spatially on the atomic scale when all charges are bound to the atom or in interatomic bonds.

Case i - longitudinal:

$$\left(E_{loc}\right)_L = E + \frac{P}{3\varepsilon_0} = -\frac{P}{\varepsilon_0} + \frac{P}{3\varepsilon_0} = -\frac{2P}{3\varepsilon_0}$$

Case ii - transversal:

$$\left(E_{loc}\right)_T = E + \frac{P}{3\varepsilon_0} = 0 + \frac{P}{3\varepsilon_0} = \frac{P}{3\varepsilon_0}$$

Thus, the local electric field is negative in the longitudinal direction, acting as a conservative type restoring force suppressing longitudinal displacements. For the transversal mode, however, the local field is positive, i.e. it acts in support of the lattice displacements.

1 c) Oppositely charged ion-pairs (±q) with c.o.m. displacements Δr, give dipole contributions $\vec{p} = q\Delta\vec{r} => \vec{P} = nq\Delta\vec{r}$. The eqns of motion are

L:

$$M\frac{d^2\Delta r}{dt^2} = qE_{loc} = -\frac{2P}{3\varepsilon_0} = -\frac{2nq^2\Delta r}{3\varepsilon_0}$$

$$=> \frac{d^2\Delta r}{dt^2} + \frac{2nq^2}{3\varepsilon_0 M}\Delta r = 0$$

T:

$$M\frac{d^2\Delta r}{dt^2} = qE_{loc} = \frac{qP}{3\varepsilon_0} = \frac{nq^2\Delta r}{3\varepsilon_0}$$

$$=> \frac{d^2\Delta r}{dt^2} - \frac{nq^2}{3\varepsilon_0 M}\Delta r = 0$$

In the case of L, the e.o.m. is that of a simple harmonic oscillator with $\omega_L = \sqrt{\frac{2nq^2}{3\varepsilon_0 M}} = \sqrt{\frac{k_L}{M}}$,

where k_L serves as a force constant.

For T, the equation yield an imaginary frequency, i.e. $\omega_T = \pm i\sqrt{\frac{nq^2}{3\varepsilon_0 M}} = \sqrt{\frac{k_T}{M}}$. While complex

frequencies may occur in general Fourier transforms, a purely imaginary frequency corresponds to life-time of some form for an exited state, i.e. $e^{-i(i\omega")t} = e^{\omega"t}$ (chose the negative root). For our simple model, however, life time concepts makes no sense. Accordingly, the only physically meaningful solution to the second equation is with $\omega_T = k_T = 0$.

In summary: $\varepsilon(0) \to \infty, \omega_T \to 0$ and $k_T \to 0$. This means that the EFFECTIVE restoring forces of the transversal mode vanishes, i.e. the lattice goes "soft", and the lattice charges may undergo spontaneous polarisation.

Phonon softening of the lattice relates to critical fluctuations in the response function (= polarisation=order parameter) taking place close to T_C (above and below). At T_C, $\omega_T = k_T = 0$, associated with a static displacement of the ions/charges, representing a symmetry braking of the high-temperature disordered and more symmetric phase, and gives the basis for an ordered phase with a lower symmetry. Such critical fluctuations and anomoalous behaviour of the response function (order param) in the vicinity of T_C is a footprint of a second order transition. In first order transitions, the response function is discontinuous at T_C but not anomalous at temperatures above and below the transition point.

2 a)

At equilibrium $f_{s.c.}$ should attain its minimum value wrt any of its variables, incl. $|\psi|$

$$\frac{\partial f_{s.c.}(T,\psi)}{\partial |\psi|} = 0 = 2(\alpha(T)\psi(r) + \beta(\mathrm{T}) \ |\psi(r)|^2 \ \psi(r) + \frac{1}{2m}(\vec{p}_{op})^2 \psi(r))$$

$$\Rightarrow -\alpha(T)\psi(r) = \beta(\mathrm{T}) \ |\psi(r)|^2 \ \psi(r) + \frac{1}{2m}(\vec{p}_{op})^2 \psi(r)$$

The n.s. => s.c. transition is a second order transition with disordered electrons above T_C ordering into Cooper-pairs. Thus, α and β should be defined such that the free energy reduces by ordering below T_C, while increasing by ordering above T_C. The standard choice for $\alpha(T)$ in a Landau second order transition is

$$\alpha(T) = \gamma \Delta T \ \text{ where } \ \gamma = \text{const} > 0 \ ; \ \Delta T = (T - T_C)$$

The α and β functions follows from a full series expansion of the free energy function, where α should collect all differential terms of second order in the order param, whereas β should collect all 4th order terms. Except for terms that are pure 2nd and 4th order expansions in ψ, all other terms collected by the two functions will be powers of ΔT.

From the Ginzburg-Landau equation, without any spatial variation of the order param, equilibrium should correspond to

$$(\alpha(T) + \beta(\mathrm{T}) \ |\psi|^2)\psi = 0$$

$$\Rightarrow \psi = 0 \ \text{ or } \ \psi = \pm \sqrt{\frac{-\alpha(T)}{\beta(T)}}$$

For the free energy density we find:

$$f_{s.c.}(T,\psi) - f_{n.s.}(T) = |\psi|^2 \ (\alpha(T) + \tfrac{1}{2}\beta(\mathrm{T}) \ |\psi|^2 \ ) = \begin{cases} 0 & \text{when } \psi = 0 \\ -\dfrac{\alpha(T)^2}{2\beta(T)} & \text{when } \psi = \pm\sqrt{\dfrac{-\alpha}{\beta}} \end{cases}$$

<u>Below T_C:</u> $\alpha(T) < 0 \Rightarrow$ Root real if $\beta(T) > 0$, and the ordered state ($\psi \neq 0$) is a possible solution
Hence, below T_C keep $\beta(T) > 0$, so that the ordered state has the lowest energy density.

<u>Above T_C:</u> $\alpha(T) > 0 \Rightarrow$ Root real if $\beta(T) < 0$, and the ordered state ($\psi \neq 0$) would become the preferred state. By retaining $\beta(T) > 0$, the root becomes imaginary, leaving the disordered state with $\psi = 0$ as the only physical solution.

Close to T_C it is also reasonable to treat β as a constant, independent of T. β collects all partial differentials of f which is to the 4th order in ψ, and close to T_C these would be assumed to be smaller and to change more modestly with T than the terms collected in α which is of 2nd order in ψ. It is not so important to account for this, and neglecting it has no consequence for the following tasks of the exam.

2 b)
The order-parameter $\psi(r) = \psi_0(r) e^{i\theta(r)}$ is a complex quantity which must contain information on the ordering of free electrons into Cooper-pairs at the n.s->s.c transition.

With only even powers in ψ in the expression for the free energy density, we can define $|\psi(r)|^2 = \psi*(r)\psi(r) = (\psi_0(r))^2 = n_{cp}(r)$, i.e. the density of Cooper pairs, and accordingly

$$\psi(r) = \sqrt{n_{cp}(r)}\, e^{i\theta(r)}$$

The current density:

$$\vec{j} = \frac{-i\hbar q}{2m}[\psi*\nabla\psi - \psi\nabla\psi*] - \frac{q^2\vec{A}}{m}\psi*\psi$$

$$= \frac{-i\hbar q}{2m}[\psi*(\nabla\psi_0 e^{i\theta} + \psi i\nabla\theta) - \psi(\nabla\psi_0 e^{-i\theta} - \psi*i\nabla\theta)] - \frac{q^2\vec{A}}{m}\psi_0^2$$

$$= \frac{-i\hbar q}{2m}[\psi_0\nabla\psi_0 + i\psi_0^2\nabla\theta - \psi\nabla\psi_0 + i\psi_0^2\nabla\theta] - \frac{q^2\vec{A}}{m}\psi_0^2$$

$$\vec{j} = \left[\frac{\hbar q}{m}\nabla\theta(r) - \frac{q^2\vec{A}}{m}\right]n_{cp}(r) = \left[\frac{\hbar e}{m_e}\nabla\theta(r) - \frac{2e^2\vec{A}}{m_e}\right]n_{cp}(r)$$

Concerning the phase:
It can be seen from the expression for the current density that the phase term relates to the local motion of Cooper-pair c.o.ms, i.e. the local superconducting current density.

2 c) Bulk superconductor => Meissner effect, no magnetic fields, $\vec{A} = 0$, and no spatial modulations, i.e. $\psi(r) = \text{const} = \sqrt{n_{cp}}$

Then, the Ginzburg-Landau eqn. gives

$$-\alpha(T) = \beta(T) \ |\psi(r)|^2 = \beta(T) \ n_{cp}$$

$$\Rightarrow |\psi(r)|^2 = n_{cp} = \frac{-\alpha(T)}{\beta(T)}$$

for a system in equilibrium at $T < T_C$

The critical field is defined as

$$\frac{1}{2}\mu_0 H_c^2(T) = \Delta u(T) = u_{n.s.}(T) - u_{s.c.}(T) = f_{n.s.}(T) - f_{s.c}(T,\psi) = \frac{\alpha(T)^2}{2\beta(T)} \quad \text{(see answer in a))}$$

$$\Rightarrow H_C(T) = \alpha(T)\sqrt{\frac{1}{\mu_0\beta(T)}}$$

3 a) Weak magnetisation in the paramagnetic phase, so we may apply Curies law:

$$\chi = \frac{\partial M}{\partial H} \approx \frac{M}{H} = \frac{C}{T}$$

The magnetisation is given by

A-site lattice: $\quad M_A T = CH_A = C(H_{ext} - \lambda M_B - \nu M_A)$

B-site lattice: $\quad M_B T = CH_B = C(H_{ext} - \lambda M_A - \nu M_B)$

At $T = T_N$ the system should undergo spontaneous magnetisation, even in the absence of external fields. Thus:

$$\begin{vmatrix} T + \nu C & \lambda C \\ \lambda C & T + \nu C \end{vmatrix} = (T + \nu C)^2 - \lambda^2 C^2 = 0$$

$$\Rightarrow \pm(T + \nu C) = \pm\lambda C, \quad \lambda C > 0$$

$$\Rightarrow T_N = C(\lambda - \nu)$$

To find the paramagnetic susceptibility of the total system, first express the total magnetisation of the two connected sublattices:

$$MT = (M_A + M_B)T = 2CH_{ext} - C(\lambda + \nu)M$$

$$\Rightarrow M = \frac{2CH_{ext}}{T + (\lambda + \nu)C}$$

Thus,

$$\chi = \frac{\partial M}{\partial H} = \frac{2C}{T + C(\lambda + \nu)} = \frac{2C}{T + \theta}, \quad \text{where } \theta = \frac{(\lambda + \nu)}{(\lambda - \nu)} T_N$$

3 b) Below the transition temperature, the two sublattices spontaneously order into two antiparallel systems, $M_A = - M_B$, so

$$H_A = -\lambda M_B - \nu M_A = (\lambda - \nu) M_A; \quad H_B = (\lambda - \nu) M_B$$

Accordingly we should use the Curie-Brillouin law, which gives us

$$M_A = \frac{1}{2} \frac{N}{V} \cdot g(JLS) J \mu_B \cdot B_J \left(\frac{g(JLS) J \mu_B \mu_0 (\lambda - \nu) M_A}{k_B T} \right)$$

$$M_B = \frac{1}{2} \frac{N}{V} \cdot g(JLS) J \mu_B \cdot B_J \left(\frac{g(JLS) J \mu_B \mu_0 (\lambda - \nu) M_B}{k_B T} \right)$$

The ½ prefactor enters since the N atoms are parted into two antiparallel spin systems.

J=1/2:

$$B_J(x) = 2\coth(2x) - \coth(x) = \frac{2(\coth^2 x + 1)}{2\coth x} - \frac{2\coth^2 x}{2\coth x} = \frac{1}{\coth x} = \tanh x$$

$$g(JLS) = \frac{3}{2} + \frac{1}{2} = 2$$

Hence

$$M_A = \frac{1}{2} n \mu_B \cdot \tanh \left(\frac{\mu_B \mu_0 (\lambda - \nu) M_A}{k_B T} \right)$$

$$M_B = \frac{1}{2} n \mu_B \cdot \tanh \left(\frac{\mu_B \mu_0 (\lambda - \nu) M_B}{k_B T} \right)$$

To find the Neel-temperature, we select one of the two sublattice systems, and let $T \to T_N$ from below. At the second order transition temperature, and in the absence of external fields, the magnetisation of each subsystem will be weak, so

For small x $\tanh x \approx x$ =>

$$M_A(T_N) \approx \frac{n \mu_B^2 \mu_0 (\lambda - \nu) M_A(T_N)}{2 k_B T_N} \Rightarrow T_N = \frac{n \mu_B^2 \mu_0 (\lambda - \nu)}{2 k_B}$$

Low-T convergence:

Set:

$$x = \frac{\mu_B \mu_0 (\lambda - \nu) M}{k_B T} \Rightarrow M = \frac{1}{2} n \mu_B \tanh(x)$$

$$\frac{M}{\frac{1}{2} n \mu_B} = \frac{M}{M_S} = \frac{T}{T_N} x \Rightarrow \frac{T}{T_N} x = \frac{M}{M_S} = \tanh x \quad \vee \quad x = \frac{T_N}{T} \frac{M}{M_S} \approx \frac{T_N}{T}$$

$$\Rightarrow M \approx M_S (1 - 2e^{-2T_N/T})$$

A spin wave approach to the temperature dependence of M gives rise to the so-called Bloch $T^{3/2}$ law, whereas the mean field approach suggests an exponential T-dependency. The Bloch $T^{3/2}$ law has been found to fit well with low temperature experimental results.

In reality neither will give an accurate description of the low temperature trend for the antiferromagnet. The mean field approach has its already mentioned deviating trend at low T for both spin systems, and the Bloch $T^{3/2}$- law is derived for a single parallel spin system with n.n. exchange only, not two exchanging antiparallel systems. It is therefore likely that the antiferromagnet require a more complicated spin wave based model.