



Department of Physics

Examination paper for TFY4245 Faststoff-fysikk, videregående kurs

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Permitted examination support material:

Alternative C:

Standard pocket calculator

K. Rottmann: Matematiske Formler (all language editions)

S. Barnett & T.M. Cronin: Mathematical Formulae

Other information:

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Some relationships that may be found useful:

Maxwell equations:

$$\begin{aligned}\nabla \times \vec{H} &= \vec{j} + \frac{\partial \vec{D}}{\partial t} & \nabla \cdot \vec{B} &= 0 \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} & \nabla \cdot \vec{D} &= \rho\end{aligned}$$

Electromagnetic wave equation:

$$\nabla^2 \vec{E} = \mu_0 \frac{\partial^2 \vec{D}}{\partial t^2}$$

Electromagnetic identities:

$$\begin{aligned}\vec{D} &= \epsilon_0 \epsilon \vec{E} = \epsilon_0 \vec{E} + \vec{P} \\ \vec{B} &= \mu_0 (\vec{M} + \vec{H})\end{aligned}$$

Curie-Brillouin relationship:

$$M = \frac{N}{V} \cdot g(JLS) J \mu_B \cdot B_J \left(\frac{g(JLS) J \mu_B \mu_0 H}{k_B T} \right)$$

with: $B_J(x) = \frac{2J+1}{2J} \coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J} \coth\left(\frac{x}{2J}\right)$

$$g(JLS) = \frac{3}{2} + \frac{1}{2} \frac{S(S+1) - L(L+1)}{J(J+1)}$$

Curies law:

$$\chi = \frac{C}{T}$$

Problem 1. Dielectrics (37,5 %).

Consider a single crystal with a two-atomic basis of oppositely charged ions, both positioned in lattice points with cubic symmetry. The material is dielectric and non-magnetic. In such systems the dielectric permittivity, ϵ , can be regarded as spatially isotropic, which leaves $\vec{D}$, $\vec{P}$ and $\vec{E}$ parallel inside the crystal. ϵ and $\vec{P}$ characterise the dielectric response of the system, and without any free charges they would generally have two main contributions: ionic displacements and/or atomic charge displacements.

The net polarization of the material can be ascribed to the sum of local displacements by a so-called local field,

$$\vec{E}_{loc} = \vec{E}_{ext} + \vec{E}_{cryst} = \vec{E}_{ext} + \vec{E}_1 + \vec{E}_2 + \vec{E}_3 = \vec{E}_{ext} - \frac{N_i \vec{P}}{\epsilon_0} + \frac{\vec{P}}{3\epsilon_0} + \vec{E}_3,$$

acting in each lattice point, with $\vec{E}_{ext}$ as the external electric field caused by charges outside the material, whereas $\vec{E}_{cryst}$ is a crystal response field comprised by the sum of all dipole contributions from inside the crystal volume, i.e.

$$\vec{E}_{cryst} = \sum_i \frac{3(\vec{p}_i \cdot \vec{r}_i) \cdot \vec{r}_i - r_i^2 \vec{p}_i}{4\pi\epsilon_0 r_i^5}$$

- a) Explain the nature of the different field components $\vec{E}_1$, $\vec{E}_2$ and $\vec{E}_3$ that expands $\vec{E}_{cryst}$, and show that for a crystal like the one considered here, $\vec{E}_3 = 0$.

The crystal is placed in air with non-zero humidity, thus if the material becomes polarized, water molecule dipoles are attracted from the air to the crystal surface where they effectively neutralize the macroscopic depolarization field.

Assume $\vec{E}_{ext} = 0$, but that $\vec{E}_{cryst}$ can attain non-zero values, e.g. due to a spontaneous polarization.

Let the dielectric field quantities inside the crystal be on the form $\{\vec{D}, \vec{E}, \vec{P}\} = \{\vec{D}_0, \vec{E}_0, \vec{P}_0\} e^{i\vec{k} \cdot \vec{r}}$.

We are interested in how $\vec{P}$ connect to the phonon modes (photon-phonon coupling), and accordingly limit ourselves to cases where ionic displacements dominate $\vec{P}$.

- b) Use the Maxwell relations to find general conditions for the directions and amplitudes of $\vec{D}$ and $\vec{E}$ in the crystal when $\vec{E}_{ext} = \vec{E}_1 = 0$. Connect the non-trivial solutions to longitudinal and transversal phonon modes, respectively, and explain why the result may only be valid in the long λ limit (long wavelength limit).

Finally, find the local fields, $\vec{E}_{loc}$, corresponding to the longitudinal and transversal modes, respectively.

In the long λ limit, lattice restoring forces acting at oppositely charged $\pm q$ neighbour ions have the same magnitude but are directed opposite to one another, and therefore cancel when considering the phonon-photon coupling as displacements of the ion-pair centre of mass (c.o.m).

- c) Set up eqns. of motion for the ion pair c.o.m. corresponding to the two phonon modes, with the local fields from b) as external forces, M as the effective mass, and Δr as the c.o.m. displacement. Deduce the eigenfrequencies associated with the longitudinal and transversal modes. How do you interpret the result?

If a spontaneous polarization like the one analysed here should appear in the vicinity of a temperature associated with a phase transition, would you expect the transition to be of first or second order ? Justify your answer.

Problem 2. Super conductivity (37,5 %)

The Ginzburg-Landau theory is a macroscopic model where superconductivity is described as a second order phase transition, but with additional terms allowing the model to retain some of the microscopic aspects of superconductivity.

Close to the phase transition at T_C , and in the absence of external fields $\vec{H}_{ext} = 0$, the Ginzburg-Landau free energy density functional for the superconducting state may be expressed as

$$f_{s.c.}(T, \psi) = f_{n.s.}(T) + \alpha(T) |\psi(r)|^2 + \frac{1}{2} \beta(T) |\psi(r)|^4 + \frac{1}{2m_e} |\vec{p}_{op} \psi(r)|^2$$

where the order parameter, ψ , is a complex quantity, $f_{n.s.}(T)$ the free energy density of the normal conducting state, and $\alpha(T) |\psi(r)|^2 + \frac{1}{2} \beta(T) |\psi(r)|^4$ constitute the Landau-terms for the order parameter. The last term represents additional kinetic energy in regions where the order parameter shows spatial variation, with $\vec{p}_{op} = -i\hbar\nabla - q\vec{A}$ as the generalised momentum operator for a charge q moving in an electromagnetic field with vector potential $\vec{A}$.

- a) Show that the equilibrium state of the system for $T < T_C$ is consistent with the Ginzburg-Landau equation, $\frac{1}{2m_e} (\vec{p}_{op})^2 \psi(r) + \beta(T) |\psi(r)|^2 \psi(r) = -\alpha(T) \psi(r)$.

Find suitable forms for the temperature dependence of the Landau parameters $\alpha(T), \beta(T)$.

- b) What is the physical nature of the order parameter? Express the order parameter in terms of an amplitude and a phase term, such that the amplitude relates to the density of the physical quantity represented by the order parameter.

Deduce an expression for the current density in the superconducting state, consistent with the Ginzburg-Landau framework.

$$\{\text{Hint: } \vec{j} = \text{Re}(\psi^* \frac{q}{m} \vec{p}_{op} \psi) = \frac{-i\hbar q}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{q^2}{m} \vec{A}(\psi^* \psi) \}.$$

Which physical information is described by the phase of the order parameter?

- c) The so-called critical magnetic field, $H_C(T)$, is defined such that the field energy density corresponds to the difference in energy densities between the normal and superconducting states. Use this information to show that the critical field for a bulk superconductor can be expressed through the Landau parameters alone.

Problem 3 Magnetism (25%).

Consider an antiferromagnetic solid with a paramagnetic response to external fields above a critical temperature, T_N , and with A and B as lattice sites favouring antiparallel alignment of the magnetic moments along the easy axis of magnetisation of the system.

In a mean field approach, using the so-called Weiss molecular field, and accounting only for nearest neighbour exchange fields, i.e. $\vec{H}_A = -\lambda \vec{M}_B$; $\vec{H}_B = -\lambda \vec{M}_A$, the susceptibility in the paramagnetic region can be expressed as $\chi = \frac{2C}{T + T_N}$, $T_N = \lambda C$, where $\lambda = \text{const} > 0$, and C is the Curie constant.

In the approach above, the A- and B-sites are treated as two separate sublattice systems with weak magnetisation by an external field in the paramagnetic region, so that each obey Curies law with $C_A = C_B = C$, but where the two systems are mutually connected via the exchange fields.

It turns out, however, that this model most often deviate significantly from experimental results, indicating that another parameter θ should replace the so-called Neel temperature, T_N , in the expression for the susceptibility. An improved Weiss model for the antiferromagnet can be constructed by accounting also for second nearest neighbour exchange, i.e internal exchange in the sublattice systems. The total exchange fields now become

$$\vec{H}_A = -\lambda \vec{M}_B - \nu \vec{M}_A; \quad \vec{H}_B = -\lambda \vec{M}_A - \nu \vec{M}_B,$$

where ν is a constant that can be positive or negative.

- a) Assume an external magnetic field, $\vec{H}_{ext}$, aligned along the easy axis of the system, and find expressions for the magnetisations, $\vec{M}_A$ and $\vec{M}_B$, of the two systems.

Determine T_N for the current model, taking into account that both sublattices should undergo spontaneous ordering at T_N also in the absence of external fields.

Show that the paramagnetic susceptibility $\chi = \frac{2C}{T + \theta}$, with $\theta = \frac{\lambda + \nu}{\lambda - \nu} \cdot T_N$

- b) Let the A and B sites be occupied by identical atoms with $J=1/2$, and apply the exchange field model above (without external magnetic field).

Show that the magnetisation of the two sublattice systems can be expressed

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

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

Use the result in to find an expression for T_N , and show that for very low T , $M(T)$ approaches the 0 K saturation moment, $M_S(0)$, as:

$$M(T) \approx M_S(0)(1 - 2e^{-2T_N/T}).$$

(Hint: For $x \rightarrow \infty$, $\tanh x$ converges towards 1 as $(1 - 2e^{-2x})$).

If we regard only one of the two sublattices and demand $\lambda - \nu > 0$, the result is practically identical to the mean field (Weiss molecular field model) ferromagnetic solution.

Compare the mean field trend at low temperatures to the trend found from ferromagnetic spin-wave based statistical mechanics models.

Would you expect any of the models to account reasonably for the low temperature trend in antiferromagnetic systems? Justify your answer.