Department of Physics

Examination paper for TFY4245 Faststoff-fysikk, videregående kurs

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Alternative C: Standard pocket calculator, K. Rottmann: Matematical Formulae (all language editions), S. Barnett & T.M. Cronin: Mathematical Formulae

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Originalen er:

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Some relationships that may be found useful:

Maxwell equations:

$$\nabla \times \vec{H} = \vec{j} + \frac{\partial \vec{D}}{\partial t} \qquad \nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \qquad \nabla \cdot \vec{D} = \rho$$

Electromagnetic wave equation:

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

Electromagnetic identities:

$$\vec{D} = \varepsilon_0 \varepsilon \vec{E} = \varepsilon_0 \vec{E} + \vec{P}$$

$$\vec{B} = \mu_0 (\vec{M} + \vec{H})$$

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 – Landau theory & ferroelectrics (33.33 %).

Let G_1 and G_2 represent the free-energy functions of the polar and non-polar phase, respectively, of a system which undergoes a ferroelectric phase transition at $T = T_C$. According to Landau theory, the free energy of a uniform system region (single domain), may be expanded as a power series, with the polarisation $P = \pm|\vec{P}|$ acting as the so-called order parameter. In the absence of external electric fields, the expansion can be represented as

$$G(P,T) = g_0(T) + g_1(T)P + \tfrac{1}{2}g_2(T)P^2 + \tfrac{1}{3}g_3(T)P^3 + \tfrac{1}{4}g_4(T)P^4 + ... + \tfrac{1}{n}g_n(T)P^n \qquad (1)\,.$$

Here, $g_i(T)$, $i = 0,..,n$, are general functions assumed to vary smoothly as functions of T.

Let $g_2(T) = \gamma(T-T_C)$, where $\gamma > 0$, and constant, and assume eqn. (1) applied to a second order ferroelectric phase transition with an ordered polar state at $T < T_C$. For a small temperature region about T_C, the series in eqn. (1) may be terminated after 4th order.

a) Assign g_0(T) such that the expansion in (1) is representative for both G_1 and G_2 close to T_C, and specify restrictions that must apply to g_1, g_3 and g_4 for the current situation. Provide explicit reasons for the restrictions you impose, and show that these lead to well defined free energy minima at both sides of T_C.

An external electric field, $\vec{E}_{ext}$, is introduced, which couples linearly to the system response variable symbolised by the order parameter in eqn. (1). Furthermore, assume the sample to be small and the spatial variation of the field to be in the long-wavelength limit, leaving $\vec{E}_{ext}$ ~ constant throughout the sample volume.

b) Introduce a term to account for the effect of the external field on the free energy expression in eqn. (1). Comparing with the results from a), discuss **briefly** how the presence of an (long wavelength) external field may affect the polarisation magnitudes associated with the energy minima above and below T_C.

   Express the dielectric susceptibility in a general situation with a non-zero external field, and use this to derive expressions for the dielectric susceptibilities above and below T_C for the situation in a) when the external field is zero.

Consider the system in a) and b) to be $BaTiO_3$ (BTO). Its ferroelectric response can be related to a dipole moment formed by a shift of the Ba^{2+} and Ti^{4+} ions relative to the O^{2-} ions (see Fig. 1). Just above T_C, BTO is cubic, with a= 4.02 Å. Below T_C, ionic displacement leads to a slight distortion of the cubic symmetry, and the lattice becomes tetragonal with the dipole moments aligned along the unique c-axis.

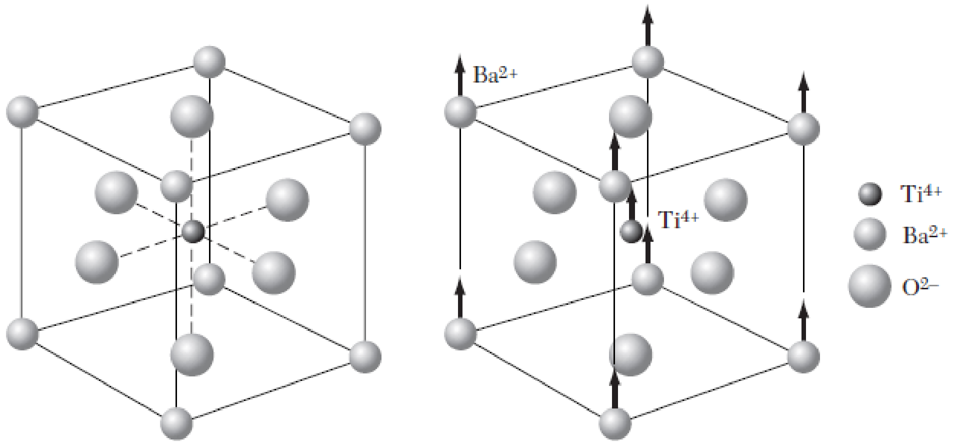

Figure 1 $BaTiO_3$ crystal structure above (left) and below (right) T_c, with positive ion shifts along *c* indicated.

The sample is cooled down from $T > T_C$ in the absence of external electric fields, and found to polarise spontaneously at $T_C = 392.1$ K. Just below T_C, at T=392 K a spontaneous polarisation of 0.04 C/m^2 is measured. Upon further cooling the polarisation rises monotonically until reaching a maximum value of 0.26 C/m^2 at 300 K.

c) Under the assumption that the relative shifts of the positive ions are identical, and that these fully account for the spontaneous polarisation when $T \le T_C$, what are the magnitudes of the relative shifts associated with the spontaneous polarisation at T= 392 K and T=300 K, respectively ?

Close to T_C the cubic distortions (i.e. ionic shifts) are small. In a first approximation the individual dipole contributions can be considered to arise from ions located in positions of nearly cubic symmetry, such that the individual microscopic polarizabilities, α_i, can be related to the mean field dielectric response function via the Classius-Mosotti relation:

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{\sum_i n_i \alpha_i}{3\varepsilon_0}$$

with n_i as the number density of dipole moments of type i.

Express the temperature dependence of the polarizability of BTO in a temperature region close to T_C. Sketch the result, and comment on its appearance, considering ionic polarizability should represent the essential critical physics in second-order displacive ferroelectric phase transitions.

From measurements we find that $\alpha_{BTO}(T_C - 0.5K) = \frac{\alpha_{BTO}(T_C)}{2}$. Use this observation to find a value for the constant γ used in a).

Problem 2. Superconductivity (33,33 %)

The superconducting current density for Cooper pairs may be written

$$\vec{j}_{c.p.}(r) = -\frac{e}{m_e} n_{c.p.}(\hbar\nabla\theta(r) + 2e\vec{A})$$

where the cooper pairs are described by a Ginzburg-Landau wave function $\psi(r) = \sqrt{n_{c.p.}}e^{i\theta(r)}$ with $n_{c.p.}$ as the cooper pair concentration, and $\theta(r)$ as a phase. $\vec{A}$ is the vector potential related to the magnetic field such that $\nabla \times \vec{A} = \vec{B}$

a) Employ Maxwell's relations to show that the London equation $\nabla^2\vec{B} = \lambda_L^{-2}B$, can be derived from the expression for superconducting current density, with λ_L as a characteristic length. What is the physical interpretation of λ_L?

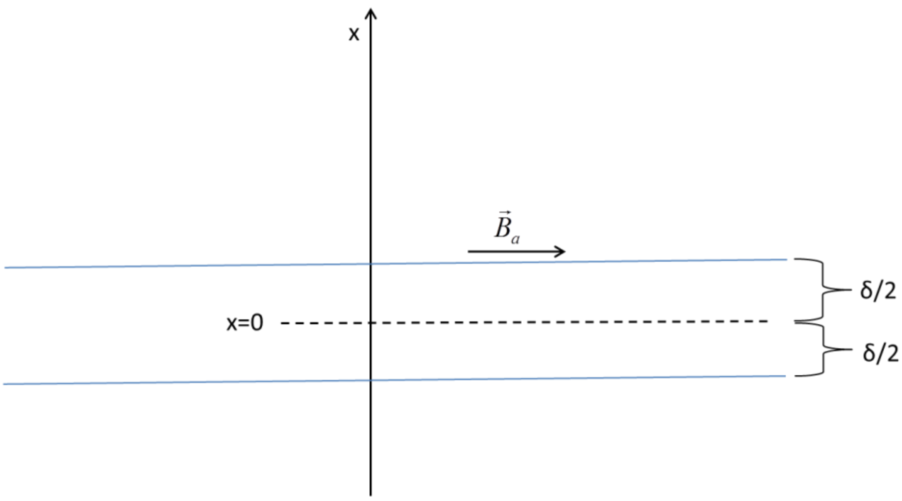

Figure 2. Cross section of superconducting plate.

b) Assume a metallic plate with thickess δ, normal to the x-axis (see fig. 2). Show that $B(x)$ inside the plate in the superconducting state is given by

$$B(x) = B_a \frac{\cosh(\frac{x}{\lambda_L})}{\cosh(\frac{\delta}{2\lambda_L})}$$

where B_a is the field outside the plate.

By decreasing the thickness to $\delta \ll \lambda_L$, the plate reduces to a thin film. Express the effective magnetization, $M(x)$, inside the plate, and show that it becomes parabolic in x as the plate thickness becomes very small.

c) Show that the free energy density of the superconductive state in the thin sheet at T= 0 K becomes

$$F_{S.C}(0,x,B_a) = F_{S.C}(0) + \frac{B_a^2}{16\mu_0\lambda_L^2}\left(\delta^2 - 4x^2\right)$$

where $F_{S.C.}(0)$ is the bulk free energy density for the superconductive state at T= 0 K.

Find the magnetic contribution to the average free energy density over the film thickness, and show that the critical field of the thin film is proportional to $(\lambda/\delta)H_C$, where H_C is the bulk critical field.

The model established in b) and c) accounts for a superconducting thin film. If $\delta \to 0$, we approach a model of a 2D superconducting sheet. When you take into consideration other physical quantities that need to be properly accounted for in the superconducting state (coherence length, current density), is it possible for a 2D sheet to be superconductive? Justify your answer.

Problem 3. Magnetism (33.33%).

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

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 λ= const > 0, and C is the Curie constant.

In the approach above, the A- and B-sites are treated as two separate sub lattice 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 anti-parallel 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 direct exchange in each of the sub-lattice systems. The modified 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 $\chi = \dfrac{2C}{T+\theta}$, with $\theta = \dfrac{\lambda+\nu}{\lambda-\nu}\cdot T_N$

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 in the antiferromagnetic phase can be expressed

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

c) Use the result in b) 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:

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

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

If we regard only one of the two sub lattices 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 well for the low temperature trend in antiferromagnetic systems? Justify your answer.