NTNU – Trondheim
Norwegian University of Science and Technology

Department of Physics

Examination paper for TFY4245 Faststoff-fysikk, videregående kurs

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Examination date: 24.05.2014

Examination time (from-to): 09:00-13:00

Permitted examination support material:

Alternative C:

Standard pocket calculator

K. Rottmann: Matematical Formulae (all language editions)

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

Other information:

The exam paper consists of three problems, each counting 1/3 of the total score.

Language: English

Number of pages: 6 (incl. front page and attachments).

Checked by:

Date Signature

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. Phonon-Photon coupling

Consider a single-crystal solid of an ionic compound with a 2 atomic basis. The solid is dielectric, non-magnetic, and for simplicity we assume its dielectric response to be isotropic, i.e. $\varepsilon_{ij}(\omega,k) \to \varepsilon(\omega,k)$.

If the solid is exposed to electromagnetic radiation, interaction may occur in the form of resonance between the electromagnetic waves and transverse optical (TO) phonons, provided that the frequency and wave vector of the external field approach those associated with the TO phonon modes.

Let $\Delta\vec{u}$, M and q represent the relative displacement, the reduced mass, and effective charge respectively, of one ion pair. The lattice acts with conservative restoring forces on the pair, which for the TO mode may be expressed $\vec{F}_{TO} = -\omega_{TO}^2 M\Delta\vec{u}$.

a) Define an equation of motion (e.o.m.) for the ion pair when it is under influence of an external electric field on the form $\vec{E}_{ext} = \vec{E}_0 \exp[i(\vec{k}\cdot\vec{r} - \omega t)]$. For simplicity, assume that the field only affects the ion pair displacement, but leaves individual ion core charge distributions unaltered.

   Assume n such ion pairs per unit volume, and show that in the long λ (wavelength) limit, the equation of motion for the individual pairs can be used to arrive at a collective e.o.m for all the ion pairs on the form:

$$(\omega_{TO}^2 - \omega^2)\vec{P} = \frac{nq^2}{M}\vec{E} \qquad (1)$$

   Is the long-λ limit assumption generally a reasonable approach to the phonon-photon coupling ? Justify your answer.

b) Employ the electromagnetic wave equation to establish another relationship between $\vec{P}$ and $\vec{E}$ in the material, and combine the result with the collective eqn. from a) to find a general dispersion relation for the phonon-photon coupling. Extract the long-λ limit behaviour by letting k -> 0, and show that the only non-trivial solution is

$$\omega = \sqrt{\omega_{TO}^2 + \frac{nq^2}{M\varepsilon_0}}$$

c) Find an expression for the long-λ dielectric function $\varepsilon(\omega, k \to 0) \approx \varepsilon(\omega)$.

   We already assumed the ion cores not to contribute to the polarisation, so the optical dielectric constant $\varepsilon(\infty) \approx 1$. Introduce the static dielectric constant $\varepsilon(0)$, and the special conditions that apply for the situation $\varepsilon(\omega) = 0$, to arrive at the so-called Lyddane-Sachs-Teller relationship:

$$\frac{\omega_{LO}^2}{\omega_{TO}^2} = \frac{\varepsilon(0)}{\varepsilon(\infty)}$$

Problem 2. Super conductivity

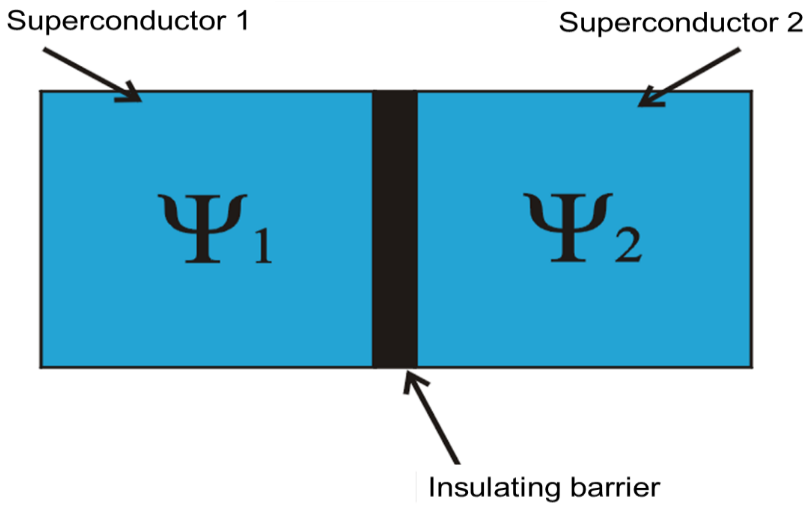

Figure 1. Josephson junction

Two superconductors are separated by a thin insulating oxide layer, as illustrated in Fig.1. Let wave functions $\psi_j = n_j^{1/2} e^{i\theta_j}$, j=1,2, describe the Cooper-pair concentrations in the two superconductors when they are far apart from one another, and assume that they both are kept at the same potential, which we set to 0, when brought together like in Fig. 1.

If the oxide layer is adequately thin, Cooper-pairs may tunnel across the barrier, between the two conductors, i.e. so-called Josephson tunnelling. If the fraction of pairs that cross the barrier is low compared to the number density, time-dependent Schrodinger equations on the form

$$i\hbar \frac{\partial \psi_1}{\partial t} = E_1\psi_1 + \hbar T \psi_2 \qquad (2)$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = E_2\psi_2 + \hbar T \psi_1 \qquad (3)$$

can be employed to describe the tunnelling. Here, T has dimension s^{-1} and is a measure of the rate of current leakage between the conductors, while E_j, j = 1,2, represents the energy per unit volume associated with Cooper pairs when superconductors 1 and 2 are separated.

a) If the two superconductors are assumed identical (i.e. of the same material, kept at the same temperature, etc. , i.e. $n_1 = n_2$ and $E_1=E_2$), show that eqns. (2) and (3) can be transformed to two complex equations with real and imaginary parts, respectively, that should obey

$$\frac{\partial n_1}{\partial t} = -\frac{\partial n_2}{\partial t} = 2Tn\sin(\theta_2 - \theta_1)$$

$$\frac{\partial \theta_1}{\partial t} = \frac{\partial \theta_2}{\partial t} = -T\cos(\theta_2 - \theta_1) - \frac{E}{\hbar}$$

and show how these relations can be used to express the current density across the barrier as $\vec{J} = \vec{J}_0 \sin(\theta_2 - \theta_1)$ where $J_0 \propto T$ and corresponds to the maximum current.
What drives current across the junction ?

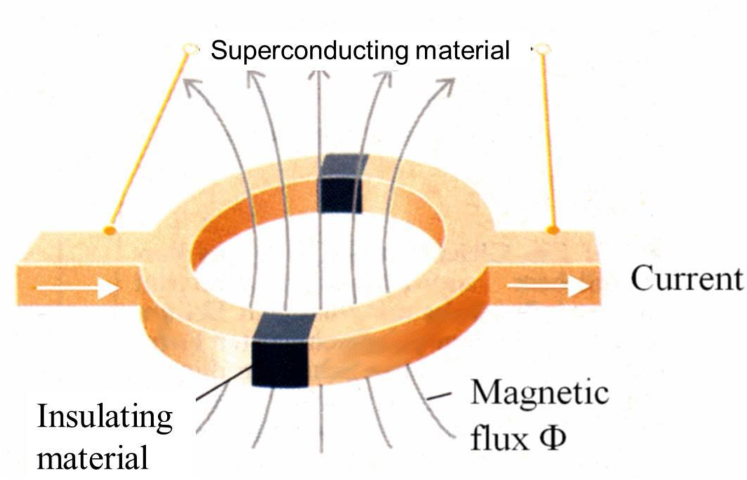

Figure 2. Superconducting current-loop containing two parallel and identical Josephson-junctions.

Two junctions like the one described above are combined into a circuit as shown in Fig 2.

a) Find an expression for the total current that runs through the loop (i.e. the two parallel junctions). (Hint: The magnetic flux through the superconducting loop can be expressed $\varphi = \varphi_0 \cdot s = \frac{\hbar \pi}{e} \cdot s, \quad s = 1, 2, ...$)
What are such devices called and what are they mainly used for ?
Concerning the functionality of the device, does it matter whether the superconductors are of type I or type II ? Justify your answer.

Problem 3 Magnetism.

Consider a solid containing two 3d transition metal ions, Mn^{2+} and Co^{3+}, with ground state electronic structures $3d^5$ and $3d^6$, respectively. The ions are arranged in a structure where formula units A = Co^{3+} and B = $Co^{3+}Mn^{2+}$ are stacked in an alternating order (ABABAB..) along the c-axis of the unit cell. Assume that the 3d orbitals of neighbouring ions overlap so that crystal field splitting in terms of quenching of the orbital angular momentum applies.

a) What are individual contributions from the two different ions to the effective number of Bohr magnetons, $p = g(JLS)(J(J+1))^{1/2}$? What would the overall p be (per formula unit AB) when the magnetic moments of A and B units are antiparallel (ferrimagnetic)?

In a mean field approach, we may express the effective magnetic field as a superposition of the external magnetic field and a so-called exchange field that handles the local interaction between neighbouring magnetic moments, i.e. $\vec{H}_{eff} = \vec{H}_{ext} + \vec{H}_{exch} = \vec{H}_{ext} + \sum_i \lambda_i \vec{M}_i$, where the sum is taken over all neighbours that contribute to the exchange.

b) Assume no external field, and find the effective fields (= exchange fields) that apply at the lattice positions occupied by A and B units, respectively. Consider nearest neighbour interactions only of the type AA and AB for A-sites, and AB and BB for B-sites, and chose exchange field coefficients such that anti-parallel ordering is energetically favourable in all directions (Energy density of magnetic fields, $dU = -\mu_0 \vec{M} d\vec{H}$)

c) Consider AB-exchange only, and find the Curie temperature, T_C, and the paramagnetic susceptibility, χ, of the system, assuming magnetisation to be weak above T_C in external fields.

Finally, sketch the magnetisation $M(T)$ of the system for $T < T_C$ in the absence of external fields. Could there be circumstances where $M(T) \to 0$?