Studentnumber:_____

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NORGES TEKNISK-NATURVITENSKAPELIGE UNIVERSITET
INSTITUTT FOR FYSIKK

Contact during the exam:
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EXAM: TFY4245 FASTSTOFF-FYSIKK VK

Monday 18. May 2009
Tid: kl 09.00-13.00

Allowed exam material: Alternative C
Standard pocket calculator
Rottman: Mathematical Formula (all language editions)
Barnett og Cronin: Mathematical Formula
English-Norwegian and/or Norwegian-English Dictionary

The exam consists of:
1. The first page (the present page) which must be delivered with answers to the multiple choice questions.
2. 3 "normal" Problems 1, 2 and 3 (Appendix A)
3. One set of multiple choice questions, Problem 4 (Appendix B)

The three "normal" problems count altogether 50%, and the multiple choice questions count altogether 50%. Only ONE of the alternatives A-D must be marked for each of the 20 multiple choice questions. Correct answer gives one point, wrong answer gives zero points.

Answers to the multiple choice questions in Appendix B:

Question	1	2	3	4	5	6	7	8	9	10
Answer										

Question	11	12	13	14	15	16	17	18	19	20
Answer										

Problem 1. Dielectrics and Ferroelectrics
1a)
Assume that we are studying a dielectric sample applying an external electric field E to it, such that the responding polarization $P = \varepsilon_0 \chi E$, where $\chi = \varepsilon-1$ is the dielectric susceptibility, ε is the dielectric constant and ε_0 is the vacuum permittivity.

• Discuss the distinction between orientational (or) P_{or} and distortional (d) P_d polarizations respectively, in dielectrics.

In a dielectric, one needs to distinguish between the externally applied field, E, and the local field, E_{loc}, in the sample. It is the local field at the site of a molecule that acts to polarize or reorient that molecule. The relation between the polarization P and the local field for monomolecular dielectrics is

$$P = P_{or} + P_d = \rho\beta E_{loc} \qquad (1.1)$$

where ρ is the particle density, and $\beta = \beta_{or} + \beta_d$ is the polarisibility.

• Discuss without entering into details, how it can be shown that for isotropic liquids and symmetric crystals

$$E_{loc} = E + P/(3\varepsilon_0) \qquad (1.2)$$

where E is the externally applied electric field, and $P/(3\varepsilon_0) = E_L$ is the so-called Lorentz-field, which represents the average (mean-field) contribution to E_{loc} acting on one molecule from all the other molecules in the sample.

• Show that for this case:

$$(\varepsilon-1)/(\varepsilon+2) = \rho\beta/(3\varepsilon_0) \qquad (1.3)$$

which is the Clausius-Mosotti equation for dielectrics.

1b)
P_{or} is related to the orientation of molecular dipoles in the dielectric. The potential energy, u, of a molecule with dipole moment p_0 in an electric field E_{loc} is:

$$u = -p_0 E_{loc} \cos\theta \qquad (1.4)$$

where θ is the angle between the dipole - direction and the E_{loc} - direction.
Defining the orientational distribution function for dipolar molecules in the dielectric as $w(\varphi,\theta)$, and thus obtaining the fraction of molecular dipoles in the angular interval $d\varphi d\theta$ as $w(\varphi,\theta)\sin(\theta)d\varphi d\theta$ (for $0<\theta<\pi$ and $0<\varphi<2\pi$), we get by using standard Boltzmann statistics i.e. $w(\theta,\varphi) \propto \exp(-u/k_B T)$, where k_B is the Boltzmann constant and T is the temperature, that:

$$P_{or} = \rho p_0 <\cos\theta> = \rho p_0 (\int d\varphi \int d\theta w(\varphi,\theta)\sin(\theta)\cos\theta)/(\int d\varphi \int d\theta w(\varphi,\theta)\sin(\theta))$$
$$= \rho p_0 \int d\theta [2\pi\sin(\theta)\cos(\theta)\exp(x\cos(\theta))]/Z \qquad (1.5)$$

where the variable $x = p_0 E_{loc}/(k_B T)$, the integral over θ run from 0 to π, the one over φ from 0 to 2π, and the normalization Z is the partition function:

$$Z = \int d\varphi \int d\theta w(\varphi,\theta)\sin(\theta) = \int d\theta [2\pi\sin(\theta)\exp(x\cos(\theta))]$$
$$= 2\pi[\exp(x)-\exp(-x)]/x \qquad (1.6)$$

• Show that for temperatures $T \gg p_0 E_{loc}/k_B$, the orientational part of the polarisibility in a dielectric can be written as:

$$\beta_{or} \approx (p_0)^2/(3k_B T) \qquad (1.7)$$

• How can this result be used in a practical experiment to measure the distortional polarisibility β_d?

1c)
• Using Equation (**1.3**), show that

$$\varepsilon_0\chi = \rho\beta/(1-\rho\beta/(3\varepsilon_0)) \qquad (1.8)$$

• Discuss what happens, and what it means in terms of physics, if β increases with decreasing T in such a way that the Lorentz-field contribution $\rho\beta/(3\varepsilon_0) = 1$ at some temperature $T = T_C$.

The simplest T-dependence one can think of for this case, is linear in T,
i.e. $\rho\beta/(3\varepsilon 0) = 1 - c(T-T_C)$, where c is a constant.

• How does χ depend on temperature for this case, for temperatures $T>T_C$?

1d)
Landau developed a phenomenological thermodynamic theory applicable to ferroelectrics (as well as other systems displaying phase transitions) describing the observations that the susceptibility diverges on approaching T_C both from above and below in T.

Landau theory assumes that near the phase transition temperature T_C, it is possible to expand the Helmholtz free energy in powers of the order parameter η (in the case of ferroelectrics $\eta = P$), thus

$$f(\eta,T) = f_0 + c_2\eta 2 + c_3\eta^3 + c_4\eta^4 + c_5\eta^5 + c_6\eta^6 + ... + c_n\eta^n + ... \qquad (1.9)$$

We assume that $c_2(T) = b(T - T_C)$, where b is a positive constant, and also assume that $c_3, c_4, c_5, c_6, ..., c_n, ...$ are constants independent of T.

• Argue that for ferroelectrics (second order phase transitions by observation): $c_3 = 0$, c_4 is positive, and one need not consider any c_n for $n > 4$, i.e $c_n = 0$ for $n > 4$.

• Sketch and discuss $f(\eta, T)$ for various T.

• Derive the temperature dependence of the order parameter for this case.

Assume that there exists an external field, X (in the case of ferroelectrics X = E), which couples linearly to the order parameter, η, i.e. an extra term $-\eta X$ must be added in the free energy expression (i.e. we use Gibbs free energy rather than Helmholtz free energy).

• Use Landau theory to derive an expression for the temperature dependence of the susceptibility both above and below T_C, thus also verifying the result obtained in **1c)**.

Problem 2. Diffusion
2a)
Diffusive motion of individual particles can formally be described by the time-dependent auto-correlation function $g_1(\mathbf{r}, t)$, defined such that the quantity $g_1(\mathbf{r}, t)d^3\mathbf{r}$ gives the probability that a particle moves during a time t from its starting point into a volume element $d^3\mathbf{r}$ which is $\mathbf{r}$ away from the starting point. $g_1(\mathbf{r}, t)$ is a probability distribution, and as such is normalized, i.e.

$$\int g_1(\mathbf{r}, t)d^3\mathbf{r} = 1 \qquad\qquad (2.1)$$

We follow Einstein, and choose to break up $g_1(\mathbf{r}, t'+t)$ into two steps, and we write

$$g_1(\mathbf{r}, t'+t) = \int g_1(\mathbf{r}-\mathbf{r}', t') \, g_1(\mathbf{r}', t)d^3\mathbf{r}' \qquad\qquad (2.2)$$

where the first step, during time t', achieves a displacement $\mathbf{r}-\mathbf{r}'$ of the particle, while the second step, in the remaining time t, brings the particle to $\mathbf{r}$.

• What is the basic assumption underlying that we write the total probability as a product of two individual probabilities representing the two steps?

• Show that Equation **(2.2)** can be rewritten (assuming $t \ll t'$ and $|\mathbf{r}'| \ll |\mathbf{r}|$) as a diffusion equation:

$$\partial g_1(\mathbf{r}, t')/\partial t = D_S \nabla^2 g_1(\mathbf{r}, t') \qquad\qquad (2.3)$$

where the self-diffusion coefficient

$$D_S = (\int g_1(\mathbf{r}', t)|\mathbf{r}'|^2 d^3\mathbf{r}')/(6t) = \langle|\mathbf{r}'|^2\rangle/(6t) \qquad\qquad (2.4)$$

represents the mean-squared displacement per unit time (divided by a factor 6).

2b)

Consider a suspension of non-interacting colloidal particles, and assume the following:

i) A particle density gradient $\nabla\rho$ resulting in a diffusive particle current described by Fick's law

$$\mathbf{j}_D = -D_S\nabla\rho \qquad\qquad (2.5)$$

ii) An external force (for example gravity) $\mathbf{f} = -\nabla u_{pot}$, where u_{pot} is the potential energy difference set by the external force, driving particle current

$$\mathbf{j}_f = \rho v\mathbf{f} = (\rho/\varsigma)\mathbf{f} \qquad\qquad (2.6)$$

where v is the mobility, and ς is the friction coefficient.

iii) At equilibrium, the particle density $\rho = \rho_{eq} = \exp(-u_{pot}/k_BT)$ according to Boltzmann statistics, where k_B is Boltzmann's constant, and T is the temperature.

Using these three assumptions:
• Show how one derives the Einstein relation:

$$D_S = k_BTv = k_BT/\varsigma \qquad\qquad (2.7)$$

Considering the result obtained in Equation (**2.4**):
• Discuss the physics contained in the Einstein relation for the "self-diffusion coefficient".

Finally:
• Discuss the difference between the "self-diffusion coefficient", D_S, and the "diffusion coefficient", D.

2c)

Equation (**2.1**), including the boundary condition $\mathbf{r}(t=0) = 0$, i.e. $g_1(\mathbf{r},t=0) = \delta(\mathbf{r})$, has the Greens-function solution

$$g_1(\mathbf{r}(t),t) = (1/(4\pi D_St))^{3/2}\exp(-|\mathbf{r}(t)|^2/(4D_St)) \qquad\qquad (2.8)$$

For non-interacting particles the time dependent structure function $S(\mathbf{q},t)$ equals the Fourier transform of $g_1(\mathbf{r}(t),t)$.

• Discuss (briefly in terms of words and equations) the theoretical basis for a light-scattering experiment which may be used to measure D_S for non-interacting colloidal particles in solution. The scattering vector $\mathbf{q}$ is the difference between the outgoing and incoming wave-vectors respectively.

Problem 3. Polymers

3a)
We define the end-to-end vector of a coiled polymer chain to be **R**.
Assume that the chain can be broken up into N_S individual uncorrelated segments $\mathbf{a}_j$ (j = 1,2,3,.....,N_S), i.e.

$$\mathbf{R} = \Sigma_j \, \mathbf{a}_j \tag{3.1}$$

For uncorrelated unrestricted $\mathbf{a}_j$ vectors, the chain geometry is equivalent to stepwise independent Brownian motion of a diffusing particle, and we can directly adopt the results obtained in Equations **(2.4)** and **(2.8)** for the Gaussian probability distribution w(**R**) for the chain end-to-end distance **R**, and its mean-squared end-to-end distance

$$R_0{}^2 = <|\mathbf{R}|^2> = \int w(\mathbf{R})R^2 4\pi R^2 dR \tag{3.2}$$

• Show that $R_0{}^2 \propto N \propto M$, where N is the degree of polymerization, and M is the chain molecular weight.

• Show that a coiled Gaussian chain is an object with fractal dimension $D_f = 2$.

3b)
The "tube model" for polymer dynamics introduced by Sam Edwards, takes entanglement effects among different chains into account in order to describe the chain dynamics in a polymer sample. This is a mean-field type model that focuses on individual chains, that includes interactions with other chains by representing them collectively as a "tube" inside which an individual chain is restricted to move, like a reptile (the de Gennes "reptation model") in linear diffusive motion (Equation **(2.7)**).

• Show that the disentanglement time, τ_d, for entangled polymer chains scales as

$$\tau_d \propto M^3 \tag{3.3}$$

3c)
Internal relaxation times such as τ_d, may be measured by means of dielectric relaxation experiments. This can be described by a general set of linear equations valid also for dielectric measurements.
Consider a physical system that is forced out of equilibrium by applying a time (t) dependent external force, $\sigma(t)$, to it. For linear response, the response field perturbation of the system is:

$$\gamma(t) = \alpha \, \sigma(t) \tag{3.4}$$

where α is a linear response function which is characteristic of the specific system under consideration.

• What do γ, α and σ represent for the dielectric case?

Assuming that after "turning off σ", the system returns to equilibrium, γ(t = ∞), at a rate, dγ(t)/dt, which increases proportionally with the magnitude of the perturbation, γ(t), we may write:

$$d\gamma(t)/dt = (\gamma(t = \infty) - \gamma(t))/\tau_d \qquad (3.5)$$

where the system characteristic time, τ_d, is the constant of proportionality between the rate and the perturbation. Equation **(3.5)** represents a simple relaxation process (Debye relaxation).

Assume, that we apply a time dependent periodic force to the system, such that:

$$\sigma(t) = \sigma_0 \exp(-i\omega t) \qquad (3.6)$$

where ω is the applied frequency, and σ_0 is the force amplitude. (i = √-1)
The resulting linear response can be written:

$$\gamma(t) = \alpha(\omega)\,\sigma(t) = \gamma_0 \exp(-i\omega t + i\delta(\omega)) \qquad (3.7)$$

where δ(ω) is the phase difference between the force and the response, and and γ_0 is the response amplitude.

• Use the above Equations in order to derive an expression for the complex frequency dependent linear response function

$$\alpha(\omega) = \gamma(t)/\sigma(t) = \alpha'(\omega) + i\alpha''(\omega) \qquad (3.8)$$

for the case of a simple relaxation process like the one in Equation **(3.5)**.

• Sketch both α'(ω) = Re(α(ω)) and α''(ω) = Im(α(ω)) for this case.

• The real and imaginary parts of the compliance are often referred to as the storage part and the loss part respectively. Discuss the physics behind this distinction.

Problem 4. Multiple choice questions

1.
The static structure factor $S(\mathbf{q})$ is a direct measure of:
a) The positions of the atoms within the unit cell?
b) The Fourier transform of the order parameter?
c) The Fourier transform of time-correlations between different particles?
d) None of the above?

2.
Which of the following types of radiation has the longest penetration depth into materials:
a) X-rays?
b) Electrons?
c) Neutrons?
d) Visible light?

3.
The order parameter for nematic order of quadrupoles is ($<\,>$ denotes an average using the appropriate orientational distribution function, and $\theta = 0$ is the director orientation):
a) $<(3\sin^2\theta-1)/2>$?
b) $<1-(3/2)\sin^2\theta>$?
c) $<\cos^2\theta>$?
d) None of the above?

4.
The order parameter for nematic order of dipoles is ($<\,>$ denotes an average using the appropriate orientational distribution function, and $\theta = 0$ is the director orientation):
a) $<(3\cos2\theta-1)/2>$?
b) $<1-(3/2)\sin^2\theta>$?
c) $<\cos^2\theta>$?
d) None of the above?

5.
In general, the isotropic to nematic phase transition is:
a) First order?
b) Second order?
c) Without order?
d) None of the above?

6.
A pure elastic solid is described by:
a) The Newtonian flow law: stress = viscosity*shear-rate
b) Hooke's law: stress = modulus*strain
c) A loss modulus that has a peak at the time characteristic for plastic flow
d) None of the above?

7.
Piezoelectricity in a material means that:
a) There is a linear relationship between elastic and magnetic fields in a material?
b) There is a non-linear relationship between the elastic and electric fields in a material?
c) There is no coupling between elastic and electro-magnetic fields in a material?
d) None of the above?

8.
Diamagnetism:
a) Diamagnetism is the term used for magnetism in materials with permanent magnetic dipoles?
b) Diamagnetism is present only ferromagnetic materials?
c) Diamagnetism is present in only in paramagnetic materials?
d) None of the above?

9.
Paramagnetism:
a) Paramagnetism is present in all materials, except in diamagnetic materials?
b) The paramagnetic susceptibility is in general very small relative to the diamagnetic susceptibility?
c) The paramagnetic susceptibility is in general negative?
d) None of the above?

10.
In the ferromagnetic state (i.e. $T<T_C$), the magnetic susceptibility, κ, generally is found to obey a power law of the form $\kappa \propto (T - T_C)^{-\gamma}$, where γ is a constant.
It is possible to show that:
a) $\gamma = 1$ is always valid for ferromagnets?
b) γ is system (i.e material) dependent for ferromagnetic transitions?
c) $\gamma = \frac{1}{2}$ is always valid for ferromagnets?
d) None of above?

11.
The superconducting Cooper pairs:
a) Are fermions?
b) Are formed by pairs of electrons bound together by exchanging phonons?
c) Are localized to within typical unit cell dimensions (~Å)?
d) None of the above?

12.
The coherence length in a superconductor is defined as:
a) The decay length for superconducting currents of Cooper pairs into the superconductor?
b) The length over which a Cooper pair is localized?
c) The decay length of an external applied magnetic field into a superconductor?
d) None of the above?

13.
Applied magnetic fields are displaced from inside type-I superconducting samples (Meissner effect). The exponential decay length (The London penetration depth) of an applied magnetic field into a type-I superconductor beneath the surface, also describes:
a) The decay length for superconducting currents of Cooper pairs in the superconductor?
b) The length over which Cooper pairs are localized?
c) The decay length for the density of Cooper pairs?
d) None of the above?

14.
The lower critical field H_{C1} in type-II superconductors describes:
a) The field for which there is complete penetration of the externally applied field in all the sample?
b) The field for which the first single flux-line is created?
c) The field for which the number of flux-lines equals the number of Cooper-pairs?
d) None of the above?

15.
The upper critical field H_{C2} in type-II superconductors describes:
a) The field for which there is complete penetration of the externally applied field in all the sample?
b) The field for which the first single flux-line is created?
c) The field for which the number of flux-lines equals the number of Cooper-pairs?
d) None of the above?

16.
The frequency positions of the Brillouin doublet peaks measured in Rayleigh-Brillouin experiments provide information about:
a) Lifetimes of pressure fluctuations?
c) Lifetimes of heat fluctuations?
b) Propagation velocities of sound waves?
d) None of the above?

17.
The frequency widths of the Brillouin doublet peaks measured in Rayleigh-Brillouin experiments provide information about:
a) Lifetimes of pressure fluctuations?
c) Lifetimes of heat fluctuations?
b) Propagation velocities of sound waves?
d) None of the above?

18.
Landau theory:
Phase transitions are often described by Landau theory starting from a free energy expansion of the form $g = g_0 + b(T - T_C)P^2 + C_3 P^3 + C_4 P^4 + C_6 P^6 - EP$, where T is the temperature and P is the order-parameter, and T_C, b, C_2, C_3, C_4, C_6 are constants.
a) Landau theory in this form is a general molecular field theory valid only for second order phase transitions independent of the values ands signs of the constants T_C, b, C_2, C_3, C_4, C_6?
b) Landau theory in this form describes second order phase transitions only when $C_3 < 0$, $C_6 = 0$ and $C_4 > 0$?
c) Landau theory in this form always describes second order phase transitions provided $C_3 = 0$?
d) None of the above?

19.
For second order phase transition, near the critical temperature T_C, critical fluctuations may become important for the observed behavior.
Which of the following statements is true?
a) Critical fluctuations are formally included in mean-field theories?
b) Critical fluctuations are caused by infinitely large restoring forces giving emergent dynamic and spontaneous regions of finite order parameter near T_C?
c) Critical fluctuations are typically restricted in size to unit cell dimensions ($\sim$Å)?
d) None of the above?

20.
The Kramers-Kronig (K-K) formulas give relations between the real and imaginary parts of generalized linear response functions, i.e. between the storage and the loss moduli respectively. The physics behind the K-K relations is:
a) That the system obeys simple Debye relaxation behaviour?
b) There is no physics behind the K-K relations, they are purely mathematical?
c) The superposition principle, i.e the system behavior may be described as a linear combination of fundamental modes?
d) None of the above?