

Studentnumber: _____

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NORGES TEKNISK-NATURVITENSKAPELIGE UNIVERSITET
INSTITUTT FOR FYSIKK

Contact during the exam:
Department of Physics
Professor Jon Otto Fossum, mob, 91139194

EXAM: TFY4245 FASTSTOFF-FYSIKK VK

Thursday 31. May 2007
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

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	11	12
Answer												

Question	13	14	15	16	17	18	19	20
Answer								

Problem 1. Fields, response functions and relaxation processes:

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: $\gamma(t) = \alpha \sigma(t)$, where α is a linear response function which is characteristic of the specific system under consideration. Assuming that the system returns to equilibrium, $\gamma(t = \infty)$, at a rate, $d\gamma(t)/dt$, which increases proportionally with the magnitude of the perturbation, $\gamma(t)$, we may write:

$$d\gamma(t)/dt = (\gamma(t = \infty) - \gamma(t))/\tau \quad (1)$$

where the system characteristic time, τ , is the constant of proportionality between the rate and the perturbation. τ contains information about the dynamics of physical processes in the system that couple to the external field σ . Equation (1) represents a simple relaxation process (Debye relaxation).

- a) We will discuss responses to general external forces for the three types of experiments listed in the following table:

Experiment type	External force $\sigma(t)$	Comment on the response $\gamma(t)$
1 Step	Step function: $\sigma(t < t_0) = 0$ and $\sigma(t \geq t_0) = \sigma_0$	$\gamma(t = \infty) = \alpha\sigma_0$
2 Pulse	δ -function: $\sigma(t) = \sigma_0\delta(t)$	$\gamma(t = \infty) = 0$
3 Dynamic	Time dependent: $\sigma(t) = \sigma_0 \exp(-i\omega t)$	$\gamma(t) = \gamma_0 \exp(-i\omega t + i\delta(\omega)) = \alpha(\omega) \sigma(t)$ ω is the applied frequency $\delta(\omega)$ is the phase difference between the force and the response σ_0 and γ_0 are force and response amplitudes respectively

- Using Equation (1), and the comments given in the table, derive and sketch in figures, expressions for $\gamma(t)$ for experiment types 1 and 2.
 - For the case of experiment type 3, derive and sketch the expression for the complex frequency dependent response function $\alpha(\omega) = \exp(i\delta(\omega)) = \gamma(t)/\sigma(t)$.
- b) Assume that we are studying a dielectric sample applying an external electric field E to it. In this case, the force defined in a) is the applied electric field $\sigma = E$, and the response of the system is the sample polarization, $\gamma = P$. The linear response function for this case is $\alpha = \epsilon_0\chi$ where $\chi = \epsilon - 1$ is the dielectric susceptibility, ϵ is the dielectric constant and ϵ_0 is the vacuum permittivity. In reality, E and P are vectors, but for simplicity we use scalar variables here. The general experiment types and general expressions derived in a) can be transferred directly to simple Debye relaxation phenomena in dielectrics, like we consider now.
- Discuss the distinction between orientational (or) P_{or} and distortional (d) P_d polarizations respectively, in dielectrics.
 - Sketch and discuss in a schematic drawing the real part of $\epsilon_0\chi$ versus frequency for a typical dielectric.

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

$$P = P_{or} + P_d = \rho\beta E_{loc}$$

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

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

$$E_{loc} = E + P/(3\epsilon_0)$$

Here E is the externally applied electric field, and $P/(3\epsilon_0) = E_L$ 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:

$$(\epsilon-1)/(\epsilon+2) = \rho\beta/(3\epsilon_0)$$

which is the Clausius-Mosotti equation for dielectrics, and also that

$$\epsilon_0\chi = \rho\beta/(1-\rho\beta/(3\epsilon_0))$$

- 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 $\rho\beta/(3\epsilon_0) = 1$ at some temperature $T = T_C$. The simplest T dependence one can think of for this case is linear in T , i.e. $\rho\beta/(3\epsilon_0) = 1 - c(T-T_C)$, where c is a constant.

- c) 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:

$$u = -p_0 E_{loc} \cos\theta$$

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 $w(\phi, \theta)$, and thus obtaining the fraction of molecular dipoles in the angular interval $d\phi d\theta$ as $w(\phi, \theta) \sin(\theta) d\phi d\theta$ (for $0 < \theta < \pi$ and $0 < \phi < 2\pi$), we get by using standard Boltzmann statistics i.e. $w(\theta, \phi) \propto \exp(-u/k_B T)$, where k_B is the Boltzmann constant and T is the temperature, that:

$$\begin{aligned} P_{or} &= \rho p_0 \langle \cos\theta \rangle = (\int d\phi \int d\theta w(\phi, \theta) \sin(\theta) \cos\theta) / (\int d\phi \int d\theta w(\phi, \theta) \sin(\theta)) \\ &= \rho p_0 \int d\theta [2\pi \sin(\theta) \cos(\theta) \exp(x \cos(\theta))] / Z \end{aligned}$$

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

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

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

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

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

Problem 2. Phase transitions and Landau theory:

Landau theory is a phenomenological thermodynamic theory describing phase transitions. This theory considers a free energy $g(\eta, T)$ of the system, where T is the temperature, and η is an order parameter which is defined to be equal to zero for temperatures above the phase transition temperature T_C . Landau theory assumes that near T_C , when η is small, it is possible to expand the free energy in powers of η , thus:

$$g(\eta, T) = g_0 - X\eta + c_2\eta^2 + c_3\eta^3 + c_4\eta^4 + c_5\eta^5 + c_6\eta^6 + \dots + c_n\eta^n + \dots$$

Here, X is an external field, which couples bilinearly to the order parameter, η , and c_n ($n = 2, 3, 4, \dots$) are constants. We generally assume based on physical arguments, that $c_2(T) = b(T - T_C)$, where b is a positive constant, and that $c_3, c_4, c_5, c_6, \dots, c_n, \dots$ are constants independent of T . g_0 is the part of the free energy that is not related to the phase transition under consideration.

a)

- What is the general meaning of, and the general definition of, an order parameter in the context of phase transitions?
- Give examples of specific order parameters (η) and their corresponding external fields (X) for some real physical systems: For example for ferroelectrics, ferromagnets, ferroelastics, nematics, dipolar nematics, superconductors, etc.

b)

- Discuss in general what is meant by “first order” and “second order” phase transitions. What do “first” and “second” refer to in this case?
- In terms of the Landau theory, consider the three cases in the following table, and for each of the three cases discuss whether the transition is of first or of second order kind.

<i>Case 1:</i> $c_3 = 0$, c_4 is positive, and $c_n = 0$ for $n > 4$
<i>Case 2:</i> $c_3 = c_5 = 0$, c_4 is negative, c_6 is positive, and $c_n = 0$ for $n > 6$
<i>Case 3:</i> c_3 is negative, c_4 is positive, and $c_n = 0$ for $n > 4$.

- Also for each of the three cases, assuming that there is no external field applied, i.e. $X = 0$, sketch and discuss (no calculations) $\eta(T)$ versus T , and also $g(\eta, T)$ versus η , for various T . Discuss the physical relevance of each of the three cases.

c)

- For *Case 1* in b), derive an expression for the temperature dependence of the equilibrium value of the order parameter $\eta_{eq}(X = 0)$, and show that for this case, the order parameter susceptibility

$$\chi(T < T_C, X=0) = -1/2 \chi(T > T_C, X=0)$$

where $\chi = d\eta/dX$ is the linear response function for application of external field X resulting in response η .

- Discuss how this $\chi(T)$ - behavior obtained from Landau theory is related to the Clausius-Mosotti equation derived in Problem 1.
- For *Case 1*, show that for the specific heat $C_v = -T(dS/dT) = -T(d^2g/dT^2)$, we can write: $C_v(T > T_C, X=0) = \text{constant}$, and that

$$C_v(T < T_C, X=0) = C_v(T > T_C, X=0) + Tb^2/(2c_4)$$

d)

- For *Case 3* in b) (also called the Landau - de Gennes expansion), derive an expression for the temperature dependence of the equilibrium value of the order parameter $\eta_{eq}(X = 0)$.

Problem 3. Polymer structure and dynamics:

- a) 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. $g_1(\mathbf{r}, t)$ is a probability distribution, and as such is normalized, i.e. $\int g_1(\mathbf{r}, t) d^3\mathbf{r} = 1$.

We follow Einstein, and choose to break up $g_1(\mathbf{r}, t + \Delta t)$ into two steps, and we write

$$g_1(\mathbf{r}, t + \Delta t) = \int g_1(\mathbf{r} - \mathbf{r}', t) g_1(\mathbf{r}', \Delta t) d^3\mathbf{r}' \quad (2)$$

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 Δt , 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) can be rewritten (assuming $\Delta t \ll t$ and $|\mathbf{r}'| \ll |\mathbf{r}|$) as a diffusion equation:

$$\partial g_1(\mathbf{r}, t) / \partial t = D_S \nabla^2 g_1(\mathbf{r}, t) \quad (3)$$

where the self-diffusion coefficient

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

represents the mean squared displacement per unit time.

- Show that D_S is a constant, and thus, that the mean squared displacement $\langle |\mathbf{r}'|^2 \rangle$ for individual diffusing particles increases linearly with time.

- b) Assume that we release a diffusing particle in origo $\mathbf{r} = 0$ at time $t = 0$, i.e. $g_1(\mathbf{r}, t=0) = \delta(\mathbf{r})$. With this starting condition, Equation (3) has the following "Green's function" solution:

$$g_1(\mathbf{r}(t), t) = (3/(2\pi \langle |\mathbf{r}|^2 \rangle))^{3/2} \exp(-3|\mathbf{r}(t)|^2 / (2\langle |\mathbf{r}|^2 \rangle)) \quad (4)$$

which then represents a Gaussian probability distribution function for the motion of a Brownian particle.

We define the end-to-end vector of a coiled polymer chain to be $\mathbf{R}$. Assume that the chain can be broken up into N_S individual uncorrelated segments $\mathbf{a}_j$ ($j = 1, 2, 3, \dots, N_S$), i.e. $\mathbf{R} = \sum_j \mathbf{a}_j$. 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 probability distribution Equation (4) as the probability distribution $w(\mathbf{R})$ for the chain end-to-end distance $\mathbf{R}$, i.e.:

$$w(\mathbf{R}) = (3/(2\pi R_0^2))^{3/2} \exp(-3R^2 / (2R_0^2))$$

where $R = |\mathbf{R}|$ and $R_0^2 = \langle |\mathbf{R}|^2 \rangle = \int w(\mathbf{R}) R^2 d^3\mathbf{R} = \int w(\mathbf{R}) R^2 4\pi R^2 dR$.

- Show that $R_0^2 = N_S \langle |\mathbf{a}_j|^2 \rangle \propto N \propto M$, where N is the degree of polymerization, and M is the chain molecular weight.
- Present an argument showing that a coiled Gaussian chain is an object with a fractal dimension $D_f = 2$.

- c) Using standard Boltzmann statistics, one may derive the Einstein relation for the self-diffusion coefficient:

$$D_S = k_B T \nu = k_B T / \zeta$$

where k_B is the Boltzmann constant, T is the temperature, ν is the particle mobility, and ζ is the friction coefficient.

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, and 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").

- Present an argument showing that the disentanglement time, τ_d , for entangled polymer chains scales as

$$\tau_d \propto M^3$$

Problem 4. Multiple choice questions:

1. The static structure factor $S(\mathbf{q})$ measured in static scattering experiments is a direct measure of:
 - a) The positions of the atoms in the unit cell?
 - b) The Fourier transform of the order parameter?
 - c) The Fourier transform of space correlations between different particles?
 - d) None of the above?
2. X-rays scatter from:
 - a) The electrons in the sample?
 - b) The neutrons in the sample?
 - c) The protons in the sample?
 - d) The photons in the sample?
3. Which of the following is NOT true regarding the cause of finite width of experimentally measured Bragg scattering peaks from a periodic structure:
 - a) A finite width may result from finite sample size, i.e. finite number of scattering planes?
 - b) A finite width may result from phonons?
 - c) A finite width may result from finite instrument resolution?
 - d) A finite width may not result from impurities or lattice defects?
4. Which of the following type of radiation has the largest penetration depth into black materials:
 - a) X-rays?
 - b) Electrons?
 - c) Neutrons?
 - d) Visible light?
5. Scanners used in Atomic Force Microscopes (AFM) are usually made from:
 - a) Ferromagnets?
 - b) Piezoelectrics?
 - c) Superconductors?
 - e) Liquid crystals?

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

7. In general, the imaginary part of a frequency dependent linear susceptibility describes:
 - a) The heat loss from the sample before any force is applied?
 - b) The loss of potential energy from the sample when the force is applied and released?
 - c) The power taken up by the sample from the applied force, and in general distributed as heat loss?
 - d) None of the above?

8. Diamagnetism:
 - a) Diamagnetism is the term used for magnetism in materials with induced electric dipoles?
 - b) The atomic diamagnetic susceptibility depends on the number of electrons in the atom?
 - c) Diamagnetism is present in only a few materials?
 - d) None of the above?

9. Paramagnetism:
 - a) Paramagnetism is present in all materials, except in diamagnetic materials?
 - b) The paramagnetic susceptibility for a sample with localized magnetic moments is inversely proportional to the temperature squared?
 - c) The paramagnetic susceptibility is in general negative?
 - d) None of the above?

10. 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 behavior.
 - b) The causality principle, i.e. no response until after the applied force?
 - c) The superposition principle, i.e the system behavior may be described as a linear combination of fundamental modes?
 - d) There is no physics behind the K-K relations, they are purely mathematical?

- 11.** In zero applied magnetic field, the size and shape distributions of Weiss domains in a ferromagnet are in general given as a result of:
- a) A competition between the diamagnetic energy and the paramagnetic energy?
 - b) A competition between the stray field energy and the earth magnetic field energy?
 - c) A competition between the stray field energy and the domain wall energy?
 - d) None of the above?
- 12.** Ferromagnetism is basically a result of:
- a) Classical interaction between magnetic dipoles?
 - b) Quantum mechanical exchange forces between spins of neighboring atoms?
 - c) Quantum mechanical exchange of phonons resulting in paired electrons?
 - d) None of the above?
- 13.** 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 included in the classical Landau theory?
 - b) Critical fluctuations are caused by infinitely small restoring forces giving emergent dynamic and spontaneous regions of finite order parameter near T_C ?
 - c) Critical fluctuations are considered to be objects with a size proportional to the lattice spacing of the material?
 - d) None of the above?
- 14.** The critical field H_c in a typical type-I superconductor is:
- a) Proportional to $(T_C - T)$?
 - b) Proportional to $(T_C - T)^2$?
 - c) Proportional to $(T_C - T)^{1/2}$?
 - d) None of the above?
- 15.** The superconducting Cooper pairs:
- a) Are bosons?
 - b) Are formed by pairs of electrons bound together by exchanging photons?
 - c) Are localized electron-pairs where the electrons in a pair typically are less than one lattice spacing apart?
 - d) None of the above?

- 16.** The coherence length in a superconductor is defined as:
- The decay length for superconducting currents of Cooper pairs into the superconductor?
 - The length over which Cooper pairs are correlated?
 - The decay length for the density of Cooper pairs?
 - The decay length of an applied magnetic field into a type-I superconductor?
- 17.** The lower critical field H_{c1} in a type-II superconductor describes:
- The field for which there is complete penetration of the externally applied field in all the sample?
 - The field for which the first single flux-line is created?
 - The field for which the number of flux-lines equals the number of Cooper-pairs?
 - None of the above?
- 18.** The rubber polymer elastic force is referred to as an entropic force. By this we mean that:
- When a polymer chain is stretched isothermally, the entropy does not change?
 - When a polymer chain is stretched isothermally, only the internal energy changes?
 - When a polymer chain is stretched isothermally, the entropy changes and the internal energy does not change?
 - None of the above?
- 19.** In a Dynamic Light Scattering (DLS) experiment, the dynamic structure factor $S(\mathbf{q}, t)$ is measured, where $\mathbf{q}$ is the scattering vector. Typical scattering curves from samples made from a dilute suspensions of Brownian diffusing colloidal spheres follow a simple relaxational behavior of the kind $S(\mathbf{q}, t) = \exp(-t/\tau(|\mathbf{q}|))$, where the relaxation time $\tau(|\mathbf{q}|) = C |\mathbf{q}|^2$. The proportionality constant C is
- $C = D_s$, the self diffusion constant?
 - $C = 1/D_s$, the inverse of the self diffusion constant?
 - $C = v$, the mobility?
 - $C = 1/\eta$, the inverse of the viscosity of the suspending liquid?
- 20.** The positions in frequency of the Brillouin doublet peaks measured in Rayleigh - Brillouin experiments provide information about:
- Lifetimes of sound waves?
 - Propagation velocities sound waves?
 - Lifetimes of heat waves?
 - Propagation velocities of heat waves?