TFY4245 Adv. solid state physics, Solutions Exam 28/5 2019

Problem 1 - Multiple choice

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
C	A	D	C	B	A	C	A	D	C	B	D	C	D	D

Problem 2 - Short answer questions

16) Differences between first and second order PTs:

In first order PTs : $\left(\frac{\partial G_0}{\partial T}\right)_{T=T_C} \neq \left(\frac{\partial G_1}{\partial T}\right)_{T=T_C} \Longrightarrow$ latent heat release, while for second order PTs $\left(\frac{\partial G_0}{\partial T}\right)_{T=T_C} = \left(\frac{\partial G_1}{\partial T}\right)_{T=T_C}$; $\left(\frac{\partial^2 G_0}{\partial T^2}\right)_{T=T_C} \neq \left(\frac{\partial^2 G_1}{\partial T^2}\right)_{T=T_C}$, so no latent heat released, but the system is discontinuous in terms of specific heat capacity (rate of change of entropy), during the PT.

In first order PTs the difference in the first order differential of the free energy allows for nucleation to occur at undercoolings below T_C. In second order transitions, conventional nucleation cannot occur - rather the system forms the ordered phase through anomalous fluctuations in the order parameter over a temperature range in the vicinity of T_C.

In second order transitions, the mean field magnitute of the order parameter is 0 at T_C, while in first order transitions the order parameter may spontaneously take on a non-zero value, so that at the transition temperature the ordered and disordered phase co-exist with both 0 and non-zero mean field values of the order param.

17) An exciton is a quasi-particle formed by a bound electron-hole pair, caused by the absorption of a photon. Excitons form in semi-conductors and insulators, and may move in the lattice as a bound charge-pair.

18) At room temperature, the magnetisation of a paramagnetic substance should be weak, so $g(JLS)J\mu_0\mu_B H \ll k_B T$, and Curies law applies. Expansion of $\coth(x)$ in small arguements, give $\coth(x) \simeq \frac{1}{x} + \frac{x}{3} - \mathcal{O}^3$. Hence, for small arguments the Brillouin function is approximated by

$$B_J(x) \simeq \frac{2J+1}{2J}\left(\frac{2J}{(2J+1)x} + \frac{(2J+1)x}{6J}\right) - \frac{1}{2J}\left(\frac{2J}{x} + \frac{x}{6J}\right)$$

$$= \frac{1}{x} + \frac{(2J+1)^2 x}{12J^2} - \frac{1}{x} - \frac{x}{12J^2} = \frac{4J(J+1)x}{12J^2} = \frac{(J+1)x}{3J}$$

Substituting $x = \frac{g(JLS)J\mu_0\mu_B H}{k_B T}$ gives

$$\chi(T) = \frac{\partial M}{\partial H} = \frac{\partial}{\partial H}\left(\frac{ng(JLS)J\mu_B(J+1)g(JLS)J\mu_B\mu_0}{3Jk_BT}H\right)$$

$$= \frac{n\mu_0\mu_B^2 g^2(JLS)J(J+1)}{3k_BT} = \frac{\mu_0\mu_B g(JLS)(J+1)M_s}{3k_BT}$$

$$\Longrightarrow M_S = \frac{3k_BT\chi(T)}{\mu_0\mu_B g(JLS)(J+1)}$$

Half-filled 4f shell gives S= 7/2, L=0, J=S, $g(JLS) = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)} = \frac{3}{2} + \frac{S(S+1)}{2S(S+1)} = 2$. Thus,

$$M_S = \frac{3 \cdot 1.38065 \cdot 10^{-23} \cdot 293 \cdot 2.78 \cdot 10^{-3}}{4\pi 10^{-7} \cdot 9.274 \cdot 10^{-24} \cdot 2 \cdot 9/2} \simeq 3.21 \cdot 10^5 \text{ A/m}$$

19) Use the Clasius-Mossotti relation from the formula sheet, and assume CaF_2 to be non-magnetic, i.e. $n^2 = c^2/v^2 = \frac{\epsilon\epsilon_0\mu_0}{\epsilon_0\mu_0} = \epsilon \Longrightarrow$

$$\frac{\epsilon - 1}{\epsilon + 2} = \frac{n^2 - 1}{n^2 + 2} = \frac{\sum n_j \alpha_j}{3\epsilon_0} = \frac{N(\alpha_{Ca^{2+}} + 2\alpha_{F^-})}{3\epsilon_0 a^3} = C,$$

with C as a constant, and N = 4 is the number of molecular units of CaF_2 in the unit cell. Entering numbers, we find

$$C = \frac{4 \cdot (5.22 \cdot 10^{-41} + 2 \cdot 1.16 \cdot 10^{-40})}{3 \cdot (5.46 \cdot 10^{-10})^3 8.8542 \cdot 10^{-12}} \simeq 0.263$$

Solving for n, we find

$$n^2 - 1 = Cn^2 + 2C \Longrightarrow n = \sqrt{\frac{2C + 1}{1 - C}} \simeq 1.44$$

20) The gradient term is obviously non-zero only in regions where the order parameter is varying spatially, whereas in the standard Laue-model for a single domain region, the mean field value of the order param is constant. A spatially varying order parameter would account for the order param state in domain walls, where e.g. the polarisation would have to revert from one direction to the other. Thus, employing the GL approach (with the appropriate term for the field energy density included) it is possible to add domain walls to the thermodynamic model, and account statistically for domain structures as well. With a time-depedent variant for the GL it is also possible to handle domain nucleation, competition between domains and domain growth.

Problem 3

a) From eqn (1), the effective microscopic field may be expressed

$$\vec{H}_{eff} = \vec{H}_{ext} - \frac{1}{g\mu_B\mu_0} \sum_{j \neq i} \Gamma(\Delta\vec{r}_{ij})\vec{S}_j.$$

In a mean field approach to the overall magnetisation, all spins $\vec{S}$ are assumed equivalent, and replaced by their thermal average value $< \vec{S} >_T$. Thus, for the mean field approximation to the effective field, with nearest neighbour direct exchange only, we find:

$$\vec{H}_{eff} = \vec{H}_{ext} - \frac{1}{g\mu_B\mu_0} \sum_{j \neq i} \Gamma(\Delta < \vec{r}_{ij} >_T) < \vec{S}_j >_T = \vec{H}_{ext} - \frac{2 < \Gamma >_T N < \vec{S} >_T}{g\mu_B\mu_0}.$$

The meanfield magnetisation is given by

$$\vec{M} = \frac{1}{V} \sum_j < \mu_j >_T = \frac{-g\mu_B}{V} \sum_j < \vec{S}_j >_T = -ng\mu_B < \vec{S} >_T .$$

Substituting $\vec{M}$ into the expression for the effective field yields

$$\vec{H}_{eff} = \vec{H}_{ext} + \lambda\vec{M} \qquad \text{with} \qquad \lambda = \frac{2 < \Gamma >_T}{n\mu_0\mu_B^2 g^2}$$

Accordingly, thermal averaging on the microscopic model yields a result consistent with the Weiss model.

b) In the paramagnetic phase, $T > T_C$, but close to the transition temperature, we assume weak magnetisation in the presence of a non-zero H_{ext}, such that Curies law does apply. We use the small argument approximation for the Brillouin function from question 18) to find

$$M = \frac{np^2\mu_B^2\mu_0}{3k_BT}(H_{ext} + \lambda M) = \frac{C}{T}(H_{ext} + \lambda M)$$

$$\Longrightarrow M(T - C\lambda) = CH_{ext} \Longrightarrow \chi = \frac{\partial M}{\partial H_{ext}} = \frac{C}{T - T_C},$$

with

$$T_C = C\lambda = \frac{ng^2S(S+1)\mu_B^2\mu_0}{3k_B}\frac{2 < \Gamma >_{T\simeq T_C}}{n\mu_0\mu_B^2g^2} = \frac{2S(S+1) < \Gamma >_{T_C}}{3k_B}$$

c)

$$M = ng\mu_BSB_S\left(\frac{gS\mu_0\mu_BH}{k_BT}\right)$$

Enter microscopic and mean field versions of H_{eff} with $H_{ext} = 0$.

Mean field:

$$M = ng\mu_BSB_S\left(\frac{gS\mu_0\mu_B\lambda M}{k_BT}\right) = ng\mu_BSB_S\left(\frac{2 < \Gamma >_T S}{n\mu_Bgk_BT}M\right)$$

Microscopic:

$$M = ng\mu_BSB_S\left(\frac{\sum_i \vec{\mu}_i\vec{H}_{eff}}{k_BT}\right) = ng\mu_BSB_S\left(\frac{- < \Gamma >_T \sum_i \vec{S}_i(\vec{S}_{i-1} + \vec{S}_{i+1})}{k_BT}\right)$$

Difference: Microscopic version retains the full energy accountancy of spin-wave, i.e. including the full distribution of spins, whereas the mean field version only holds for the net behaviour. In the microscopic version it is therefore possible to handle changes/fluctuations of the spin wave, such as e.g. inversion of the spin-orientation through domain walls, the role of defects/imperfections, etc. Nevertheless, for the net behaviour in single domains the mean field version gives a pretty good description.

Problem 4

a) By expressing the continuity relation in terms of Fourier components, we find

$$-i\omega\rho_{ind} + i\vec{k}\vec{j}_{ind} \Longrightarrow \rho_{ind} = \frac{\vec{k}\vec{j}_{ind}}{\omega} = \frac{\sigma}{\omega}\vec{k}\vec{E}$$

while Gauss law gives:

$$\imath\vec{k}\vec{E} = \frac{\rho_{tot}}{\epsilon_0} \Longrightarrow \rho_{tot} = i\epsilon_0\vec{k}\vec{E}$$

Substituting for the charge densities in the expression for the dielectric response function, we arrive at

$$\epsilon(\vec{k},\omega) = 1 - \frac{\rho_{ind}(\vec{k},\omega)}{\rho_{tot}(\vec{k},\omega)} = 1 - \frac{\sigma(\vec{k},\omega)\vec{k}\vec{E}}{i\omega\epsilon_0\vec{k}\vec{E}} = 1 + \frac{i\sigma(\vec{k},\omega)}{\omega\epsilon_0}$$

b) In the long-wavelenght limit, the response function from a) becomes

$$\epsilon(\omega) = 1 + \frac{i\sigma(\omega)}{\omega\epsilon_0} = 1 + \frac{i\sigma_0}{\epsilon_0\omega(1 - i\omega\tau)} = 1 + \frac{\sigma_0(i - \omega\tau)}{\epsilon_0\omega(1 + \omega^2\tau^2)} = 1 - \frac{\sigma_0\tau}{\epsilon_0(1 + \omega^2\tau^2)} + i\frac{\sigma_0}{\epsilon_0\omega(1 + \omega^2\tau^2)} \tag{1}$$

For the plasma system, we set up an equation of motion, with losses added

$$m\frac{d^2\vec{x}}{dt^2} = -\frac{m}{\tau}\frac{d\vec{x}}{dt} - e\vec{E} - e\vec{v}_x \times \mu\vec{H} \Longrightarrow\ -\omega^2m + i\omega m/\tau)\vec{x} = -e\vec{E} - e\vec{v}_x\vec{H}$$

Thus, collectively the plasma motion becomes

$$\vec{P} = -ne\vec{x} = -\frac{ne^2\tau}{m\omega(\omega\tau - i)}\left[\vec{E} + \mu\frac{\hbar k}{m}\hat{x} \times \vec{H}\right] \simeq \frac{ne^2\tau}{m\omega(\omega\tau - i)}\vec{E},$$

where we have used the long wavelength limit $\vec{k} \to 0$ when ignoring a net magnetic contribution. From the electromagnetic identities on the formula sheet, we find

$$\epsilon(\omega) = 1 + \frac{P}{\epsilon_0 E} = 1 - \frac{ne^2\tau}{m\epsilon_0\omega(\omega\tau - i)} = 1 - \frac{ne^2\tau(\omega\tau + i)}{m\epsilon_0\omega(\omega^2\tau^2 + 1)} = 1 - \frac{ne^2\tau^2}{m\epsilon_0(\omega^2\tau^2 + 1)} - i\frac{ne^2\tau}{m\epsilon_0\omega(\omega^2\tau^2 + 1)} \qquad (2)$$

In the plasma frequency regieme, (typically from UV and above), $\omega\tau \gg 1$. We may therefore approximate the denominators of eqn (1) and (2) by $(\omega^2\tau^2 + 1) \approx \omega^2\tau^2$
The results are:

$$\epsilon(\omega) = 1 - \frac{\sigma_0}{\epsilon_0\omega^2\tau} + i\frac{\sigma_0}{\epsilon_0\omega^3\tau^2} \qquad (1b)$$

$$\epsilon(\omega) = 1 - \frac{ne^2}{m\epsilon_0\omega^2} - i\frac{ne^2}{m\epsilon_0\omega^3\tau} = 1 - \frac{\omega_p^2}{\omega^2} - i\frac{\omega_p^2}{\omega^2}\frac{1}{\omega\tau} \qquad (2b)$$

In the last eqn, we have introduced the plasma frequency. Equating the expressions for the response functions, we find from the real parts:

$$\omega_p = \sqrt{\frac{\sigma_0}{\epsilon_0\tau}} \simeq 3.3 \cdot 10^{16}\mathrm{s}^{-1}$$