Exam: Introduction to Condensed Matter Theory

Friday, April 1, 2016

The total number of points is 50. Do not forget to write your name and the student number on the first sheet. Good luck.

1. **Kinetic energy of ions in a crystal** A crystal with a Bravais lattice is formed by ions of mass M. The momentum operator of the n-th ion, $\boldsymbol{P}_n$, is expressed in terms of the phonon creation and annihilation operators by

$$\boldsymbol{P}_n = \frac{1}{i\sqrt{N}} \sum_{q\lambda} \boldsymbol{e}_{q\lambda} \sqrt{\frac{\hbar M \omega_{q\lambda}}{2}} \left(b_{q\lambda} e^{i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}} - b^\dagger_{q\lambda} e^{-i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}} \right), \tag{1}$$

   (a) Show that the average kinetic energy of the ion is given by

$$\left\langle \frac{\boldsymbol{P}_n^2}{2M} \right\rangle = \frac{1}{2N} \sum_{q\lambda} \hbar\omega_{q\lambda} \left(n_{q\lambda} + \frac{1}{2} \right); \tag{2}$$

   where $n_{q\lambda}$ is the average number of phonons with the wave vector $\boldsymbol{q}$ and polarization λ. [4 points]

   (b) Find the average kinetic energy in the Debye model at zero temperature, assuming for simplicity that the phonon speed is independent of polarization: $\omega_{q\lambda} = vq$. Express the average kinetic energy in terms of the $k_B\Theta$, where k_B is the Boltzmann constant and Θ is the Debye temperature. [3 points]

   (c) Find the average kinetic energy at high temperatures, $T \gg \Theta$. [3 points]

   Hint: Use the Bose-Einstein distribution to find an approximate expression for $n_{q\lambda}$ *at* $k_B T \gg \hbar\omega_{q\lambda}$.

2. **Elastic energy of a cubic crystal:** A crystal lattice that belongs to the cubic class 23 is invariant under 120°-rotations around body diagonals of the cube, e.g. $3_{[111]} = (y,z,x)$, and 180°-rotations around the crystal axes axes: $2_x = (x,-y,-z)$, $2_y = (-x,y,-z)$ and $2_z = (-x,-y,z)$. Find the most general expression for the harmonic lattice energy in terms of the components of the strain tensor,

$$u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$

   [10 points]

3. **Spin chain with anisotropic interactions**

Consider a spin chain with the lattice constant a. The spin Hamiltonian has the form,

$$\hat{H} = -\sum_n \left[J_\perp \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y \right) + J_\parallel S_n^z S_{n+1}^z \right]. \tag{3}$$

Assuming that $S \gg 1$ and using Holstein-Primakoff transformation from spin to boson operators,

$$\begin{aligned} S_n^- = S_n^x - iS_n^y &= a_n^\dagger \sqrt{2S - a_n^\dagger a_n}, \\ S^+ = S_n^x + iS_n^y &= \sqrt{2S - a_n^\dagger a_n}\, a_n, \\ S_n^z = S - a_n^\dagger a_n, & \end{aligned} \tag{4}$$

find the dependence of the magnon energy on the magnon wave vector **k**.

[10 points]

Hint: Keep only the terms of second and first orders in S in the boson Hamiltonian. In this approximation $S_n^- \to a_n^\dagger \sqrt{2S}$ *and* $S_n^+ \to a_n \sqrt{2S}$.

4. **Tight-binding model**

Conduction electrons in a crystal with a cubic lattice in the magnetic field along the z-axis, $\boldsymbol{B} = B_z \hat{z}$, are described by the tight-binding Hamiltonian ,

$$\begin{aligned} H = & - t \sum_{n\sigma} \left[c_{n\sigma}^\dagger (c_{n+x,\sigma} + c_{n+y,\sigma} + c_{n+z,\sigma}) + (c_{n+x,\sigma}^\dagger + c_{n+y,\sigma}^\dagger + c_{n+z,\sigma}^\dagger) c_{n\sigma} \right] \\ & - \mu B_z \sum_n \left(c_{n\uparrow}^\dagger c_{n\uparrow} - c_{n\downarrow}^\dagger c_{n\downarrow} \right), \end{aligned} \tag{5}$$

where n denotes sites of the cubic lattice with the lattice constant a, $\sigma = \uparrow, \downarrow$ is the spin projection, the site $n + x$ is the nearest neighbor of the site n along the x-direction, e.g. $\boldsymbol{X}_{n+x} = \boldsymbol{X}_n + a\hat{x}$, t is the hopping amplitude and μ is the electron magnetic moment.

Find the dependence of the energy of the conduction electron, $\varepsilon_{\boldsymbol{k}\sigma}$, on the wave vector $\boldsymbol{k}$ and the spin projection σ. [10 points]

5. **Kramers-Kronig relations**

   (a) The real and imaginary parts of the dielectric susceptibility, $\chi'(\omega)$ and $\chi''(\omega)$, satisfy

$$\chi'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} d\xi \frac{\chi''(\xi)}{\xi - \omega}. \tag{6}$$

   What is the physical origin of this relation? [2 points]

(b) Prove that the Kramers-Kronig relation (6) can be re-written as the principle value integral over positive frequencies:

$$\chi'(\omega) = \frac{2}{\pi} P \int_0^{+\infty} d\xi \frac{\xi \chi''(\xi)}{\xi^2 - \omega^2}. \quad (7)$$

[2 points]

Hint: How is $\chi''(-\omega)$ related to $\chi''(\omega)$?

(c) The optical absorption spectrum of a material is:

$$\chi''(\omega) = \begin{cases} 0, & \text{for } 0 < \omega < \Omega_1, \\ A, & \text{for } \Omega_1 < \omega < \Omega_2, \\ 0, & \text{for } \omega > \Omega_2, \end{cases} \quad (8)$$

i.e. the imaginary part of the dielectric susceptibility, $\chi''(\omega)$, is constant between Ω_1 and Ω_2 and is zero otherwise. Find the dielectric function at zero frequency, $\varepsilon(\omega = 0)$. [3 points]

Hint: Outside the interval $\Omega_1 < \omega < \Omega_2$ the principle value integral becomes a normal integral. $\varepsilon = 1 + 4\pi\chi$.

(d) Show that for $\omega \gg \Omega_2$, $\varepsilon(\omega) \approx 1 - \frac{\omega_p^2}{\omega^2}$. Find the expression for the 'plasma frequency', ω_p. [3 points]