Freddie Hendriks

Exam: Introduction to Condensed Matter Theory

Thursday, April 4, 2019

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. **Average ion density in a cubic crystal** Consider a crystal with a Bravais lattice formed by ions of mass M. The coordinate operator of the n-th ion in the crystal is $\hat{\boldsymbol{X}}_n = \boldsymbol{X}_n^{(0)} + \hat{\boldsymbol{Q}}_n$, where $\hat{\boldsymbol{Q}}_n$, is the displacement of the ion from its minimial-energy position, $\boldsymbol{X}_n^{(0)}$. For a harmonic lattice,

$$\left\langle e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{Q}}_n} \right\rangle = e^{-W}, \tag{1}$$

where $W = \frac{1}{2}\left\langle (\boldsymbol{k}\cdot\hat{\boldsymbol{Q}}_n)^2 \right\rangle$ is the Debye-Waller factor.

(a) Show that for crystal with a simple cubic lattice

$$W = \frac{1}{6}\boldsymbol{k}^2 \left\langle \hat{\boldsymbol{Q}}^2 \right\rangle. \tag{2}$$

[2 points]

Hint: Use symmetry arguments.

(b) Calculate the mean square displacement, $\langle \hat{\boldsymbol{Q}}^2 \rangle$, at zero temperature in the Debye model with the phonon dispersion, $\omega_{q\lambda} = \mathrm{v}q$, for all phonon polarizations, $\lambda = 1,2,3$. Express the result in terms of the Debye frequency, ω_D. [4 points]

Hint:

$$\hat{\boldsymbol{Q}}_n = \frac{1}{\sqrt{N}} \sum_{q\lambda} \boldsymbol{e}_{q\lambda} \left[\frac{\hbar}{2M\omega_{q\lambda}}\right]^{\frac{1}{2}} \left(\hat{b}_{q\lambda} e^{i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}} + \hat{b}^\dagger_{q\lambda} e^{-i\boldsymbol{q}\cdot\boldsymbol{X}_n^{(0)}} \right). \tag{3}$$

(c) The density operator of point-like ions at a point $\boldsymbol{x}$ is formally defined as

$$\hat{n}(\boldsymbol{x}) = \sum_n \delta^{(3)}(\boldsymbol{x} - \hat{\boldsymbol{X}}_n). \tag{4}$$

Show that the average ion density in a crystal with a simple cubic lattice is given by

$$\langle \hat{n}(\boldsymbol{x}) \rangle = \sum_n f(\boldsymbol{x} - \boldsymbol{X}_n^{(0)}) \tag{5}$$

with

$$f(\boldsymbol{x}) = \left(\frac{3}{2\pi\langle\hat{Q}^2\rangle}\right)^{3/2} \exp\left(-\frac{3\boldsymbol{x}^2}{2\langle\hat{Q}^2\rangle}\right). \tag{6}$$

[4 points]

Hint: How about calculating first the average Fourier transform of the ion density,

$$\hat{n}_{\boldsymbol{k}} = \int d^3x e^{-i\boldsymbol{k}\cdot\boldsymbol{x}} \hat{n}(\boldsymbol{x}),$$

and then inverse Fourier transform?

Useful relations: $\frac{a}{2}\boldsymbol{k}^2 + i\boldsymbol{b}\cdot\boldsymbol{k} = \frac{a}{2}(\boldsymbol{k} + i\frac{\boldsymbol{b}}{a})^2 + \frac{\boldsymbol{b}^2}{2a}$ *and* $\int_{-\infty}^{+\infty} dx e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$.

2. **Elastic energy of lead molybdate:** The crystal lattice of lead molybdate (wulfenite, see Fig. 1), $PbMoO_4$, belongs to the tetragonal crystal class $4/m$ (C_{4h}). The generators of the point group are the 90°-rotation around the z axis, $4_z = (-y, x, z)$, and the horizontal mirror, $m_z = (x, y, -z)$.

   (a) Is $PbMoO_4$ invariant under the following symmetry operations? Explain your answer.

      i. $2_z = (-x, -y, z)$ (180°-rotation around the z axis) [1 point]

      ii. $m_y = (x, -y, z)$ (y-mirror) [1 point]

      iii. $I = (-x, -y, -z)$ (inversion) [1 point]

   (b) Give the most general expression for the harmonic lattice energy of this tetragonal crystal in terms of the components of the strain tensor $u_{\alpha\beta}$. [7 points]

3. **Spin waves in a ferromagnetic chain:** Consider a spin chain with the Hamiltonian

$$H = \sum_n \left[-J\mathbf{S}_n \cdot \mathbf{S}_{n+1} - \frac{K}{2}(S_n^z)^2 - \mu\mathscr{H} S_n^z\right], \qquad J, K, \mu\mathscr{H} > 0, \tag{7}$$

where $\mathbf{S}_n$ denotes spin at the site n with the coordinate $X_n = na$, a being the lattice constant. The first, second and third terms in Eq.(7) describe, respectively, ferromagnetic exchange interactions, single-ion anisotropy and Zeeman energy ($\mathscr{H}$ is the magnetic field applied in the z direction). The anisotropy term with $K > 0$ favors spins parallel or antiparallel to the z axis.

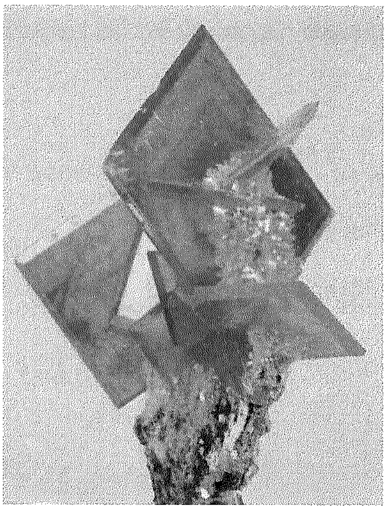

FIG. 1: Wulfenite.

(a) Using the Dyson-Maleev transformation from spin to boson operators,

$$\begin{cases} S_n^- = S_n^x - iS_n^y \;=\; \sqrt{2S}a_n^\dagger, \\ S_n^+ = S_n^x + iS_n^y \;=\; \sqrt{2S}\left(1 - \frac{a_n^\dagger a_n}{2S}\right) a_n, \\ \qquad\quad S_n^z \;=\; S - a_n^\dagger a_n, \end{cases} \tag{8}$$

find the magnon energy, ε_k, as a function of the magnon wave vector k, for $S \gg 1$. [7 points]

Hint: In the $S \gg 1$ limit, the fourth-order terms in the boson operators a_n and $a_n^\dagger$ can be neglected. $\mathbf{S}_1 \cdot \mathbf{S}_2 = S_1^z S_2^z + \frac{1}{2}\left(S_1^+ S_2^- + S_1^- S_2^+\right)$. *Write the boson Hamiltonian in the momentum space.* $a_k = \frac{1}{\sqrt{N}} \sum_n e^{-ikX_n} a_n$.

(b) Find the two first terms of the expansion of ε_k in powers of $(ka)^2$, for $ka \ll 1$. Explain why the magnon spectrum has a gap. [3 points]

4. **Tight-binding model with a longer range hopping:** Consider a conducting chain described by the Hamiltonian,

$$H = -\sum_{n\sigma} \sum_{m \neq 0} t_{n,n+m} \left(c_{n\sigma}^\dagger c_{n+m,\sigma} + c_{n+m,\sigma}^\dagger c_{n\sigma} \right), \tag{9}$$

where $c_{n,\sigma}$ is the operator annihilating electron with the spin projection $\sigma = \uparrow, \downarrow$ at the site n. The hopping amplitude decreases exponentially with the distance between the sites:

$$t_{n,n+m} = t_0 e^{-\kappa |X_{n+m} - X_n|} = t_0 e^{-\kappa a |m|}, \quad m = \pm 1, \pm 2, \ldots, \tag{10}$$

where a is the lattice constant, $X_n = na$ is the coordinate of the site n and κ is the inverse hopping range.

(a) Find the energy, ε_k, of electron with the wave vector k. Try to express ε_k in terms of elementary functions. [6 points]

Hint: Re-write the Hamiltonian (9) in terms of the Bloch wave operators, $c_{k\sigma}$:

$$\begin{cases} c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_n e^{-ikX_n} c_{n\sigma}, \\ \\ c_{n\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ikX_n} c_{k\sigma}, \end{cases} \tag{11}$$

where N is the total number of lattice sites. To perform the summation over the hopping distances, do it separatly for positive and negative m.

(b) Near the bottom of the electron band,

$$\varepsilon_k \approx \varepsilon_0 + \frac{\hbar^2 k^2}{2m_*}, \quad \text{for} \quad |k|a \ll 1, \tag{12}$$

where m_* is the effective electron mass. Find m_* and discuss the two limiting cases: $\kappa a \gg 1$ and $\kappa a \ll 1$. [4 points]

Hint: For $\kappa a \gg 1$, it is convenient to introduce the nearest-neighbor hopping amplitude, $t_1 = t_0 e^{-\kappa a}$.

5. **Kramers-Kronig relations, plasmon and sum rule**

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

$$\chi'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} d\xi \frac{\chi''(\xi)}{\xi - \omega}, \tag{13}$$

where $P\int$ is the principal value integral. What is the physical origin of this relation? [1 point]

(b) Prove that the Kramers-Kronig relation (13) can be re-written as the principle value integral over positive frequencies:

$$\chi'(\omega) = \frac{2}{\pi} P \int_{0}^{+\infty} d\xi \frac{\xi \chi''(\xi)}{\xi^2 - \omega^2}. \tag{14}$$

[3 points]

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

(c) Show that the imaginary part of the dielectric susceptibility of metal, $\chi''(\omega)$, obeys the sum rule,

$$\int_{0}^{\infty} d\omega\omega\chi''(\omega) = \frac{\omega_p^2}{8},$$

where ω_p is the plasmon frequency. [6 points]

Hint: Use asymptotic form of the dielectric function, $\varepsilon(\omega) = 1 + 4\pi\chi(\omega)$, *of metal at high frequencies.*