Midterm Exam Trial- "Quantum Matter" (NS-371B)

April 5, 2012
Duration of the exam: 2 hours

1. Use a separate sheet for every exercise.

2. Write your name and initials in all sheets, on the first sheet also your address and your student ID number.

3. Write clearly, unreadable work cannot be corrected.

4. You are NOT allowed to use any kind of books or lecture notes. A list with some useful formulas is given at the end of the exam sheet.

Spin Waves

1. Ferromagnetic materials have excitations called "spin waves" or "magnons", corresponding to oscillations in the magnetization direction that (classically) behave as waves. Their dispersion is

$$\varepsilon_{\mathbf{k}} = J\left[3 - \cos(k_x a) - \cos(k_y a) - \cos(k_z a)\right] \ , \qquad (1)$$

where J is the so-called "spin stiffness" and a is the lattice constant. The aim here is to understand how the heat capacity depends on the temperature.

(a) (1.5) Given the fact that spin waves obey the Planck distribution function, determine their contribution to the heat capacity at low temperatures and in three dimensions. *Hint:* expand the dispersion for small k_x, k_y, k_z, determine the internal energy U, and then determine the heat capacity C. Write the integral in terms of dimensionless variables and call it I_{3D}.

(b) (1.5) Same as (a), but now in one and two dimensions. Guess the expression for ε_k in one and two dimensions, looking at Eq.(1).

(c) (1.0) How is the temperature dependence for spin-waves in d-dimensions?

Phonon dispersion in graphene

2. Carbon-based materials have always attracted a lot of scientific interest. Recently, in 2004, experimental physicists succeeded in isolating *graphene*,
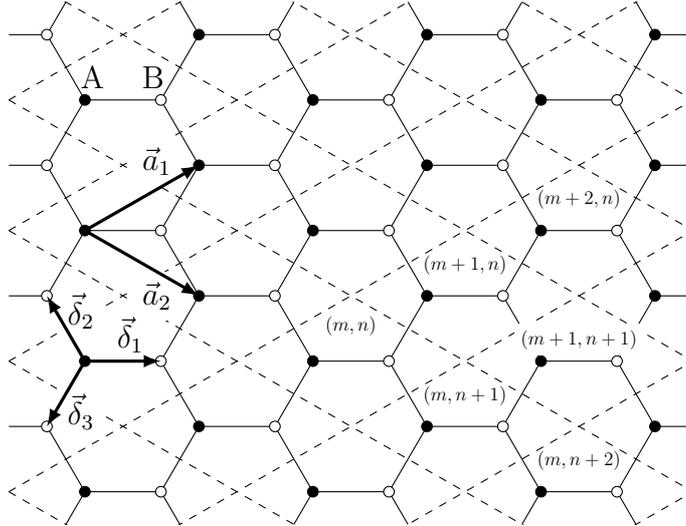
Figure 1: Graphene lattice

a two dimensional layer of carbon atoms, arranged in a regular hexagonal lattice, see Fig. 1.

Although graphene only consists of carbon atoms, the unit cell contains two atoms, which we call A and B. These atoms have to be treated independently, since the bonds to their nearest neighbours are arranged differently. In the figure, the graphene lattice is drawn, with atoms of type A drawn as solid circles and those of type B as open circles. The dashed parallelograms are the unit cells, which we label by (m, n) (shown on the figure). The vectors to the nearest neighbours of an A atom are

$$\vec{\delta_1} = a(1,0), \qquad \vec{\delta_2} = \tfrac{1}{2}a(-1, \sqrt{3}), \qquad \vec{\delta_3} = \tfrac{1}{2}a(-1, -\sqrt{3}),$$

where a is the distance between two neighbouring carbon atoms.

The lattice vectors indicate how the unit cells are arranged. These are given by

$$\vec{a_1} = \tfrac{1}{2}a(3, \sqrt{3}), \qquad \vec{a_2} = \tfrac{1}{2}a(3, -\sqrt{3}).$$

The positions of the atoms are expressed conveniently in terms of these lattice vectors. The positions of the A and B atom of the (m, n)-th unit cell are given by

$$\vec{x}_{A\,m,n} = m\,\vec{a_1} + n\,\vec{a_2}, \qquad \vec{x}_{B\,m,n} = \vec{x}_{A\,m,n} + \vec{\delta_1}.$$

In this problem, we consider the *in-plane* phonon modes of graphene. These modes are characterised by plane waves. In this case, the displacements of

the atoms are given by

$$\vec{u}_{\text{A}\,m,n}(t) = \vec{u}_{0\,\text{A}} \exp(i\vec{k} \cdot \vec{x}_{\text{A}\,m,n} - i\omega\,t),$$
$$\vec{u}_{\text{B}\,m,n}(t) = \vec{u}_{0\,\text{B}} \exp(i\vec{k} \cdot \vec{x}_{\text{B}\,m,n} - i\omega\,t),$$

where $\vec{k}$ is the wave vector, ω is the frequency, and $\vec{u}_{0\,\text{A}}$ and $\vec{u}_{0\,\text{B}}$ are two constant vectors indicating the amplitude and direction of the displacements.

(a) (2.0) Write down the equations of motion for this system. Use M for the mass of a carbon atom, and K for the spring constant of the bond between two carbon atoms. *Hint:* Write first the equations of motion in terms of the displacements and their derivatives, and then express x_{B} in terms of x_{A} (and vice versa) using $\vec{\delta}_1$, $\vec{\delta}_2$, and $\vec{\delta}_3$ in the expression for the displacements. Show that

$$-\frac{M}{K}\omega^2\vec{u}_{0\,\text{B}} = \vec{u}_{0\,\text{A}}f(-\vec{k}) - 3\vec{u}_{0\,\text{B}}$$
$$-\frac{M}{K}\omega^2\vec{u}_{0\,\text{A}} = \vec{u}_{0\,\text{B}}f(\vec{k}) - 3\vec{u}_{0\,\text{A}}$$

with $f(\vec{k}) = \mathrm{e}^{i\vec{k}\cdot\vec{\delta}_1} + \mathrm{e}^{i\vec{k}\cdot\vec{\delta}_2} + \mathrm{e}^{i\vec{k}\cdot\vec{\delta}_3}$.

(b) (1.0) Starting from the equations of motion, it is possible to show (don't do it) that the dispersion is given by

$$[\omega(\vec{k})]^2 = \frac{3K}{M}\left(1 \pm \sqrt{\frac{|f(\vec{k})|^2}{9}}\right).$$

How many modes are there per unit cell? Why? What is the total number of in-plane modes in a graphene sample of N atoms?

(c) (1.5) Due to the linear behaviour of the dispersion of the acoustic modes for low momenta $|\vec{k}|$, this system is described well by the Debye model in the low-$|\vec{k}|$ limit. Expand the acoustic modes around a minimum and derive the speed of sound v_{s}.

(d) (1.5) The Debye frequency ω_{D} is the frequency for which $\int_0^{\omega_{\text{D}}} g(\omega)\mathrm{d}\omega$ equals the total number of modes. Here, $g(\omega)$ is the density of states. Give an expression for the density of states for this system. Subsequently, calculate the Debye frequency for the in-plane modes. Give your answer in units of a/L, where L^2 is the area of the system.

Formulas

- Maxwell-Boltzmann distribution: $g(\varepsilon) \propto \exp(-\varepsilon/k_B T)$

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- Gibbs distribution:
$$P_i = \frac{\exp\{\beta(\mu N_i - E_i)\}}{\mathcal{Z}}, \qquad \mathcal{Z} = \sum_i \exp\{\beta(\mu N_i - E_i)\}$$

- For the different ensembles:
$$\Omega = e^{\beta TS}, \qquad Z = e^{-\beta F}, \qquad \mathcal{Z} = e^{-\beta \Phi_G},$$
where S is the entropy, T is the temperature, $\beta = (k_B T)^{-1}$, $F = -k_B T \ln Z$ is the Helmholtz function, and $\Phi_G = -k_B T \ln \mathcal{Z} = F - \mu N = -pV$ is the grand-potential.

- Recall the usual relations from quantum mechanics:
$$E = \hbar\omega, \qquad p = \hbar k, \qquad E = p^2/2m$$

- Photons:
$$\omega = ck, \qquad k = 2\pi/\lambda, \qquad c = \lambda\nu$$
$$E = \hbar kc = pc$$

- Planck distribution:
$$f(E) = \frac{1}{e^{\beta E} - 1}$$

- Fermi-Dirac and Bose-Einstein distributions:
$$\ln \mathcal{Z} = \pm \sum_i \ln\left(1 \pm e^{\beta(\mu - E_i)}\right)$$
$$f(E) = \frac{1}{e^{\beta(E-\mu)} \pm 1},$$
where the sign $+$ stands for fermions and the sign $-$ stands for bosons.

- Polylogarithm function $\mathrm{Li}_n(z)$:
$$\int_0^\infty dx \frac{x^{n-1}}{z^{-1}e^x \pm 1} = \mp\Gamma(n)\mathrm{Li}_n(\mp z), \qquad \mathrm{Li}_n(1) = \zeta(n),$$
where ζ is the Riemann zeta-function, and $\Gamma(n) = (n-1)!$ for n a positive integer.
$$\mathrm{Li}_1(z) = \ln\left(\frac{1}{1-z}\right)$$

- Gaussian integral:
$$\int_{-\infty}^{+\infty} dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}}$$