Midterm Exam- Solutions
Thermal Physics 2 (NS-355B) 2009

2D Bose-Einstein Condensation

1. (a) The particle number of the 2D Bose gas is

$$N = \int_0^\infty d\epsilon D_2(\epsilon) N_{BE}(\epsilon)$$
$$= \frac{Am}{2\hbar^2\pi} \int_0^\infty \frac{d\epsilon}{\exp(\beta(\epsilon - \mu)) - 1}$$

Substitute $x = \exp(\beta\epsilon)$ to arrive at

$$N = \frac{Am}{2\hbar^2\pi} \int_1^\infty \frac{dx}{\beta x} \frac{1}{\zeta x - 1}$$
$$\text{where } \zeta = e^{-\mu\beta},$$
$$= \frac{Am}{2\hbar^2\pi\beta} \ln\left(\frac{\zeta}{\zeta - 1}\right)$$
$$= -\Lambda_{th}^{-2} A \ln(1 - \exp(\beta\mu)).$$

Dividing both sides by the area A we obtain,

$$\Lambda_{th}^2 n = -\ln(1 - \exp(\beta\mu)). \tag{1}$$

(b) For every value of the degeneracy parameter $\Lambda_{th}^2 n$ we can find a corresponding chemical potential. In the three dimensional case this is not possible when $\Lambda_{th}^3 n > 2.612$ above which Bose condensation takes place.

(c) The chemical potential of an ideal gas in three dimensions can be calculated by inverting $N(V, T, \mu)$. The number of particles is easily calculated from,

$$N = \int_0^\infty d\epsilon\, D_3(\epsilon) N_{MB}(\epsilon, \mu, T)$$
$$= \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty d\epsilon\, \sqrt{\epsilon} e^{-\beta(\epsilon - \mu)}$$

Substitute $x = \sqrt{\epsilon}$ to arrive at

$$
\begin{aligned}
N &= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} e^{\mu\beta} \int_0^\infty dx\, 2x^2 \exp(-\beta x^2) \\
&= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} 2e^{\mu\beta}\left(-\frac{\partial}{\partial\beta}\int_0^\infty dx\, \exp(-\beta x^2)\right) \\
&= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} e^{\mu\beta}\left(-\frac{\partial}{\partial\beta}\sqrt{\frac{\pi}{\beta}}\right) \\
&= V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} e^{\mu\beta}.
\end{aligned}
$$

Inverting the above equation yields,

$$
\mu = k_B T \ln\left(\Lambda_{th}^3 n\right). \tag{2}
$$

Spin Waves

2. (a) To derive the temperature dependence of the heat capacity for spin waves in a ferromagnet in the low temperature limit, we expand the dispersion relation for small k_x, k_y, k_z

$$
\hbar\omega_{\mathbf{k}} = J\left[3 - \cos\left(k_x a\right) - \cos\left(k_y a\right) - \cos\left(k_z a\right)\right] \approx \frac{Ja^2 k^2}{2}.
$$

This gives for the temperature dependence of the internal energy

$$
\begin{aligned}
U &= \frac{1}{(2\pi/L)^3}\int 4\pi k^2 \left(\frac{Ja^2 k^2}{2}\right)\frac{1}{e^{Ja^2\beta k^2/2} - 1}\mathrm{d}k \\
&\propto \beta^{-5/2}\int \frac{x^4}{e^x - 1}dx.
\end{aligned}
$$

Thus the specific heat depends on the temperature in the following way

$$
C \propto T^{3/2}.
$$

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(b) For spin waves in a two dimensional system, the dispersion relation reads

$$\hbar\omega_{\mathbf{k}} = J\left[2 - \cos\left(k_x a\right) - \cos\left(k_y a\right)\right] \approx \frac{Ja^2 k^2}{2}.$$

The internal energy therefore scales with the temperature as

$$
\begin{aligned}
U &= \frac{1}{(2\pi/L)^2}\int 2\pi k \left(\frac{Ja^2 k^2}{2}\right)\frac{1}{e^{Ja^2\beta k^2/2} - 1}\mathrm{d}k \\
&\propto \beta^{-4/2}\int \frac{x^3}{e^x - 1}dx.
\end{aligned}
$$

The specific heat for spin waves in the low temperature limit in two dimension is given by

$$C \propto T^1.$$

Similarly, in a one dimensional system we have

$$\hbar\omega_k = J\left[1 - \cos\left(ka\right)\right] \approx \frac{Ja^2 k^2}{2}.$$

The internal energy scales with temperature as

$$
\begin{aligned}
U &= \int \left(\frac{Ja^2 k^2}{2}\right)\frac{1}{e^{Ja^2\beta k^2/2} - 1}\mathrm{d}k \\
&\propto \beta^{-3/2}.
\end{aligned}
$$

The specific heat in this case scales as

$$C \propto T^{1/2}.$$

(c) Note that the low temperature behavior of the specific heat for phonons goes as T^d, where d is the dimension of the system. However, for spin waves the specific heat is proportional to $T^{d/2}$.

Phonons in graphene

(a) We write the equations of motion for the atoms of type A and B for the unit cell (m, n). The neighbours of the atom A in unit cell (m, n) are the B atoms

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in the unit cells (m, n), $(m-1, n)$, and $(m, n-1)$. The neighbours of the atom B in unit cell (m, n) are the A atoms in the unit cells (m, n), $(m+1, n)$, and $(m, n+1)$. The force of one bond, exerted onto an atom 1 by a neighbouring atom 2 is given by $K(\vec{u}_2 - \vec{u}_1)$. The total force on an atom is the (vectorial) sum of the three forces associated with the bonds with its neighbours. This sum is equal to its mass times the acceleration. Hence, we have

$$M\ddot{\vec{u}}_{\text{A}\,m,n} = K\left[(\vec{u}_{\text{B}\,m,n} - \vec{u}_{\text{A}\,m,n}) + (\vec{u}_{\text{B}\,m-1,n} - \vec{u}_{\text{A}\,m,n}) + (\vec{u}_{\text{B}\,m,n-1} - \vec{u}_{\text{A}\,m,n})\right]$$

$$M\ddot{\vec{u}}_{\text{B}\,m,n} = K\left[(\vec{u}_{\text{A}\,m,n} - \vec{u}_{\text{B}\,m,n}) + (\vec{u}_{\text{A}\,m+1,n} - \vec{u}_{\text{B}\,m,n}) + (\vec{u}_{\text{A}\,m,n+1} - \vec{u}_{\text{B}\,m,n})\right],$$

for the atoms A and B (respectively) of the unit cell (m, n).

The next step is to substitute the plane waves into the equations of motion. For the equation for atom A, we will divide out common factor $\exp(i\vec{k} \cdot \vec{x}_{\text{A}\,m,n} - i\omega t)$. In other words, we will write the exponentials in $\vec{u}_{\text{B}\,m,n}$, $\vec{u}_{\text{B}\,m-1,n}$, $\vec{u}_{\text{B}\,m,n-1}$ in terms of $\exp(i\vec{k} \cdot \vec{x}_{\text{A}\,m,n} - i\omega t)$, the exponential in $\vec{u}_{\text{A}\,m,n}$. We have

$$e^{i\vec{k}\cdot\vec{x}_{\text{B}\,m,n}-i\omega t} = e^{i\vec{k}\cdot(\vec{x}_{\text{B}\,m,n}-\vec{x}_{\text{A}\,m,n})}e^{i\vec{k}\cdot\vec{x}_{\text{A}\,m,n}-i\omega t} = e^{i\vec{k}\cdot\vec{\delta}_1}e^{i\vec{k}\cdot\vec{x}_{\text{A}\,m,n}-i\omega t},$$

$$e^{i\vec{k}\cdot\vec{x}_{\text{B}\,m,n-1}-i\omega t} = e^{i\vec{k}\cdot(\vec{x}_{\text{B}\,m,n-1}-\vec{x}_{\text{A}\,m,n})}e^{i\vec{k}\cdot\vec{x}_{\text{A}\,m,n}-i\omega t} = e^{i\vec{k}\cdot\vec{\delta}_2}e^{i\vec{k}\cdot\vec{x}_{\text{A}\,m,n}-i\omega t},$$

$$e^{i\vec{k}\cdot\vec{x}_{\text{B}\,m-1,n}-i\omega t} = e^{i\vec{k}\cdot(\vec{x}_{\text{B}\,m-1,n}-\vec{x}_{\text{A}\,m,n})}e^{i\vec{k}\cdot\vec{x}_{\text{A}\,m,n}-i\omega t} = e^{i\vec{k}\cdot\vec{\delta}_3}e^{i\vec{k}\cdot\vec{x}_{\text{A}\,m,n}-i\omega t},$$

using the nearest-neighbour vectors $\vec{\delta}_1$, $\vec{\delta}_2$, and $\vec{\delta}_3$. Hence the (vectorial) equation of motion of the A atom is

$$-M\omega^2\vec{u}_{0\,\text{A}} = K\left[\vec{u}_{0\,\text{B}}e^{i\vec{k}\cdot\vec{\delta}_1} - \vec{u}_{0\,\text{A}} + \vec{u}_{0\,\text{B}}e^{i\vec{k}\cdot\vec{\delta}_2} - \vec{u}_{0\,\text{A}} + \vec{u}_{0\,\text{B}}e^{i\vec{k}\cdot\vec{\delta}_3} - \vec{u}_{0\,\text{A}}\right].$$

For the B atom, the vectors to the nearest neighbours are $-\vec{\delta}_1$, $-\vec{\delta}_2$, and $-\vec{\delta}_3$. Hence, we may derive the equation of motion for the B atom from that of the A atom by swapping A with B and vice versa, and by replacing all $\vec{\delta}_i$ by $-\vec{\delta}_i$. We find

$$-M\omega^2\vec{u}_{0\,\text{B}} = K\left[\vec{u}_{0\,\text{A}}e^{-i\vec{k}\cdot\vec{\delta}_1} - \vec{u}_{0\,\text{B}} + \vec{u}_{0\,\text{A}}e^{-i\vec{k}\cdot\vec{\delta}_2} - \vec{u}_{0\,\text{B}} + \vec{u}_{0\,\text{A}}e^{-i\vec{k}\cdot\vec{\delta}_3} - \vec{u}_{0\,\text{B}}\right].$$

Dividing both sides of the equations of motion by K, and writing $f(\vec{k}) = e^{i\vec{k}\cdot\vec{\delta}_1} + e^{i\vec{k}\cdot\vec{\delta}_2} + e^{i\vec{k}\cdot\vec{\delta}_3}$, we find

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

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

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(b) There are four modes per unit cell, namely the acoustic mode (with the $-$ sign in the dispersion relation) and the optical mode (with the $+$ sign), both in two polarisation directions. The fact that there are four modes, despite the system having only one type of atom and two polarisation directions, comes from the fact that the A and B atoms are effectively different, since their neighbours are arranged differently, as argued in the introduction of the exercise.

Since the unit cell has two atoms, the total number of in-plane modes in the system is twice the number of atoms, i.e., equal to $2N$.

Extra note: If one allows for vibrations in a third direction, perpendicular to the plane, as is the case if we embed graphene into a three-dimensional space, then there are two more modes.

Extra; proof of dispersion relation:

In the equations of motion (3), we split $\vec{u}_{0\,\mathrm{A}}$ and $\vec{u}_{0\,\mathrm{B}}$ into of their x, y-components. Subsequently, we write the resulting four equations in matrix form, as

$$
\begin{pmatrix}
\frac{M\omega^2}{K} - 3 & 0 & f(\vec{k}) & 0 \\
0 & \frac{M\omega^2}{K} - 3 & 0 & f(\vec{k}) \\
f(-\vec{k}) & 0 & \frac{M\omega^2}{K} - 3 & 0 \\
0 & f(-\vec{k}) & 0 & \frac{M\omega^2}{K} - 3
\end{pmatrix}
\begin{pmatrix}
u_{0\,\mathrm{A}\,x} \\
u_{0\,\mathrm{A}\,y} \\
u_{0\,\mathrm{B}\,x} \\
u_{0\,\mathrm{B}\,y}
\end{pmatrix}
=
\begin{pmatrix}
0 \\
0 \\
0 \\
0
\end{pmatrix}. \tag{4}
$$

This equation has to be satisfied for nonzero $(u_{0\,\mathrm{A}\,x}, u_{0\,\mathrm{A}\,y}, u_{0\,\mathrm{B}\,x}, u_{0\,\mathrm{B}\,y})$. Hence, the matrix must be singular, i.e., its determinant must be zero. This condition reads

$$
\left[\left(\frac{M\omega^2}{K} - 3 \right)^2 - f(\vec{k})f(-\vec{k}) \right]^2 = 0. \tag{5}
$$

From this expression, we solve

$$
\left(\frac{M\omega^2}{K} - 3 \right) = \pm\sqrt{|f(\vec{k})|^2},
$$

using that $f(\vec{k})f(-\vec{k}) = f(\vec{k})(f(\vec{k}))^* = |f(\vec{k})|^2$. Then, we read off that

$$
\omega^2 = \frac{K}{M} \left(3 \pm \sqrt{|f(\vec{k})|^2} \right) = \frac{3K}{M} \left(1 \pm \sqrt{\frac{|f(\vec{k})|^2}{9}} \right). \tag{6}
$$

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Extra note on the result: From the matrix in equation (4) and subsequently from the square in solution (5) it becomes apparent that the solution of the dispersion, equation (6) has two copies. These copies can be associated to the x- and y-polarisations. There is no coupling between the x and y components (see (4)), so that the dispersion (6) has two copies for each of the sign choices ($-$ for acoustic and $+$ for optical). This leads to the four modes.

The argument that the *square* in ω^2 of equation (6) is responsible for two solutions for the acoustic mode and two solutions for the optical mode is not valid. In other words, for counting the number of modes, the frequencies ω and $-\omega$ should be regarded as *the same mode*, or one needs to regard only the positive solutions.

(c) First it is useful to expand the function $f(\vec{k})$

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

$$\approx 3 - \frac{1}{2}(\vec{k}\cdot\vec{\delta}_1)^2 - \frac{1}{2}(\vec{k}\cdot\vec{\delta}_2)^2 - \frac{1}{2}(\vec{k}\cdot\vec{\delta}_3)^2 \quad = 3 - \frac{3}{4}a^2k^2,$$

where the definition of the vectors δ_i was used in the last line. Thus the term $|f(\vec{k})|^2$ is

$$|f(\vec{k})|^2 = 9\left(1 - \frac{a^2k^2}{4}\right)^2.$$

From this it follows that, considering only the acoustic mode (i.e. taking the minus sign in the definition of ω),

$$\omega \approx \sqrt{\frac{3K}{M}\left(1 - \left(1 - \frac{a^2k^2}{4}\right)\right)} = \sqrt{\frac{3K}{4M}}ak.$$

The speed of sound is defined by $\omega = v_s k$ and thus

$$v_s = \sqrt{\frac{3K}{4M}}a.$$

(d) The integral up to the Debye frequency must equal the total number of modes $2N$. First we need to calculate the density of states. In terms of the momentum it is

$$g(k)\mathrm{d}k = 2 \times \frac{2\pi k}{(2\pi/L)^2}\mathrm{d}k = \frac{L^2}{\pi}\mathrm{d}k,$$

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where the factor $2\pi k \mathrm{d}k$ is the area of a momentum shell of thickness $\mathrm{d}k$ and the factor of two is due to the two polarization directions of the modes. In terms of the energy the density of states is

$$g(\omega)\mathrm{d}\omega = g(k)\mathrm{d}k = \frac{L^2}{\pi}\frac{\omega}{v_s}\frac{\mathrm{d}\omega}{v_s} = \frac{L^2\omega}{\pi v_s{}^2}\mathrm{d}\omega.$$

The integral is thus

$$\int\limits_0^{\omega_D}\frac{L^2\omega}{\pi v_s{}^2}\mathrm{d}\omega = \frac{L^2}{2\pi v_s{}^2}\omega_D{}^2 = 2N.$$

This gives for the Debye frequency

$$\omega_D = \sqrt{4\pi N}\frac{v_s}{L} = \sqrt{\frac{3NK\pi}{M}}\frac{a}{L}.$$

This equation can be further simplified by relating the number of particles to the ratio of the system size to the cell size. In each cell we have two carbon atoms, therefore the number of atoms follows from

$$\frac{N}{2} = \frac{L^2}{|\vec{a_1}||\vec{a_2}|\sin\theta} = \frac{2L^2}{3\sqrt{3}a^2},$$

where we used that $|\vec{a_1}| = |\vec{a_2}| = \sqrt{3}a$ and due to the hexagonal structure the angle between the vectors is $\theta = 60°$. Rewriting gives $\frac{L^2}{a^2} = \frac{3\sqrt{3}N}{4}$. Insering this into the Debye frequency gives

$$\omega_D = 2\sqrt{\frac{\pi K}{\sqrt{3}M}}.$$