Midterm Exam- Solutions
Quantum Matter (NS-371B) 2012

1. Magnons in Antiferromagnets

1. We use $\cos x \simeq 1 - x^2/2$ to approximate the dispersion:

$$\varepsilon_k \simeq (-J) \cdot ka. \tag{1}$$

The internal energy in 1D can be calculated in the usual way using the Planck distribution:

$$U = \sum_k \varepsilon_k \frac{1}{e^{\beta\varepsilon_k} - 1} = \frac{L}{2\pi} \int_0^\infty dk \frac{(-J) \cdot ka}{e^{\beta(-J)\cdot ka} - 1} \tag{2}$$

$$\overset{k \to k/(-J\beta a)}{=} \frac{L}{2\pi} \frac{(k_B T)^2}{-Ja} \int_0^\infty \frac{k dk}{e^{\beta k} - 1} = \frac{L}{2\pi} \frac{(k_B T)^2}{-Ja} I_{1D}. \tag{3}$$

By definition, $C = \partial U / \partial T$ and thus

$$C = \frac{L}{2\pi} \frac{2k_B^2 T}{-Ja} I_{1D}. \tag{4}$$

2. The expressions for the energy in two and three dimensions are

$$\varepsilon_k^2 = (-J)^2 \left[2 - \cos^2(k_x a) - \cos^2(k_y a)\right] \simeq (-Ja)^2 \cdot (k_x^2 + k_y^2) \tag{5}$$

and

$$\varepsilon_k^2 = (-J)^2 \left[3 - \cos^2(k_x a) - \cos^2(k_y a) - \cos^2(k_z a)\right] \simeq (-Ja)^2 \cdot (k_x^2 + k_y^2 + k_z^2), \tag{6}$$

respectively.

Proceeding analogously to 1D, in 2D we have

$$U = \sum_{k_x, k_y} \varepsilon_k \frac{1}{e^{\beta\varepsilon_k} - 1} = \frac{A}{(2\pi)^2} \int_{-\infty}^\infty dk_x dk_y \frac{(-Ja) \cdot \sqrt{k_x^2 + k_y^2}}{e^{\beta(-Ja)\cdot\sqrt{k_x^2+k_y^2}} - 1} \tag{7}$$

$$= \frac{A}{2\pi} \int_0^\infty k dk \frac{(-Ja) \cdot k}{e^{\beta(-Ja)\cdot k} - 1} \overset{k \to \frac{k}{(-J\beta a)}}{=} \frac{A}{2\pi} \frac{(k_B T)^3}{(-Ja)^2} \int_0^\infty \frac{k^2 dk}{e^{\beta k} - 1} = \frac{A}{2\pi} \frac{(k_B T)^3}{(-Ja)^2} I_{2D}. \tag{8}$$

and

$$C = \frac{A}{2\pi} \frac{3k_B^3 T^2}{(-Ja)^2} I_{2D}. \tag{9}$$

Finally, we calculate U and C in three dimensions:

$$U = \sum_{k_x,k_y,k_z} \frac{\varepsilon_k}{e^{\beta\varepsilon_k}-1} = \frac{V}{(2\pi)^3}\int_{-\infty}^{\infty} dk_x dk_y dk_z \frac{(-Ja)\cdot\sqrt{k_x^2+k_y^2+k_z^2}}{e^{\beta(-Ja)\cdot\sqrt{k_x^2+k_y^2+k_z^2}}-1} \tag{10}$$

$$= \frac{2V}{(2\pi)^2}\int_0^{\infty} k^2 dk \frac{(-Ja)\cdot k}{e^{\beta(-Ja)\cdot k}-1} \overset{k\to\frac{k}{(-J\beta a)}}{=} \frac{2V}{(2\pi)^2}\frac{(k_BT)^4}{(-Ja)^3}\int_0^{\infty}\frac{k^3 dk}{e^{\beta k}-1} \tag{11}$$

$$= \frac{2V}{(2\pi)^2}\frac{(k_BT)^4}{(-Ja)^3} I_{3D}. \tag{12}$$

and

$$C = \frac{2V}{(2\pi)^2}\frac{4k_B^4T^3}{(-Ja)^3} I_{3D}. \tag{13}$$

3. From the prior calculations it is obvious that the temperature dependence of the heat capacity in d-dimensions is $C \sim T^d$. The reason for that is the fact that the angular integral yields k^{d-1} in d-dimensions, while the dispersion is always such that $\varepsilon_k \sim k$, where k is the radial coordinate (corresponding to momentum) in the spherical coordinate system.

   As we have calculated in the exercise series 4, the temperature dependence of phonon heat capacity is the same.

2. 2D Bose-Einstein Condensation

1. The density of states in 2D is given by

$$D_2(\epsilon) = \frac{mA}{2\pi\hbar^2}\,, \qquad D_2(k) = \frac{A}{2\pi}k \tag{14}$$

   such that

$$D_2(\epsilon)d\epsilon = D_2(k)dk\,. \tag{15}$$

   The particle number of the 2D Bose gas is

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

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

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

Dividing both sides by the area A we obtain,

$$\Lambda_{th}^2 n = -\ln(1 - \exp(\beta\mu)). \tag{16}$$

2. For every value of the degeneracy parameter $\Lambda_{th}^2 n$ we can find a corresponding chemical potential because the equation can always be inverted. Remember that $\mu < 0$, hence $z = e^{\beta\mu}$ such that $0 < z < 1$ which makes the right hand side always positive and unbounded. Since the n in the formula is the density for the particles in the excited states and the equation is always consistent, as we just said, no BEC occurs. In the three dimensional case this is not possible when $\Lambda_{th}^3 n > 2.612$ above which Bose condensation takes place.

   Another way to see it is the following: let's consider the case of condensation, i.e. a macroscopic occupation of the ground state, which means that $z \to 1^-$. In this case we can inspect the formula and see that the right hand side diverges to $+\infty$ Then, the left hand side must diverge, and thus we need that $T \to 0$ (because n cannot diverge): there is no critical temperature, or in other words, the only critical temperature is the trivial one $T = 0$ because, as you would expect, at zero temperature particles occupy only the ground state.

3. 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,

$$\begin{aligned}
N &= \int_0^\infty d\epsilon\, D_3(\epsilon) N_{MB}(\epsilon, \mu, T) \\
&= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\epsilon\,\sqrt{\epsilon}e^{-\beta(\epsilon-\mu)}
\end{aligned}$$

   The density of states is given by

$$D_3(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\epsilon}\,, \qquad D_3(k) = \frac{V}{2\pi^2}k^2\,. \tag{17}$$

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,

$$\mu = k_B T \ln\left(\Lambda_{th}^3 n\right). \tag{18}$$

3. Heat capacity of liquid ^{4}He

1. The free energy can be written as

$$\begin{aligned}
F &= -k_B T \int \ln(1+n)\frac{d^3p}{(2\pi\hbar)^3} \\
&= -k_B T \int \ln\left[1+\frac{1}{e^{\beta\epsilon}-1}\right]\frac{d^3p}{(2\pi\hbar)^3} \\
&= -\frac{4\pi k_B T}{(2\pi\hbar)^3}\int \ln\left[1+\frac{1}{e^{\beta p c_1}-1}\right] p^2 dp \\
&= -\frac{4\pi k_B T}{(2\pi\hbar)^3}\frac{1}{\beta^3 c_1^3}\int \ln\left[1+\frac{1}{e^{x}-1}\right] x^2 dx \\
&\propto (k_B T)^4
\end{aligned}$$

2. The entropy can be found from the free energy, which has the following temperature dependence

$$S = -\frac{\partial F}{\partial T} \propto T^3.$$

Furthermore, the specific heat can be obtained by using $dE = TdS$ (for constant volume)

$$C_V = \frac{\partial E}{\partial T} = T\frac{\partial S}{\partial T} \propto T^3.$$

3. The Bose-Einstein distribution reduces to the Boltzmann distribution in the limit $\Delta \gg k_B T$ since

$$n = \left[e^{\beta\left(\Delta + \frac{(p-p_0)^2}{2\mu_r}\right)} - 1 \right]^{-1} \approx \left[e^{\beta\left(\Delta + \frac{(p-p_0)^2}{2\mu_r}\right)} \right]^{-1} = e^{-\beta\epsilon_r}.$$

Using a similar approximation the free energy of the ideal Bose gas reduces to the Boltzmann free energy

$$F = -k_B T \int \ln\left[1 + e^{-\beta\epsilon_r}\right] \frac{d^3p}{(2\pi\hbar)^3} \approx -k_B T \int e^{-\beta\epsilon_r} \frac{d^3p}{(2\pi\hbar)^3},$$

where we used that $\ln(1+x) \approx x$.

4. The free energy of the roton gas is given by

$$\begin{aligned}
F &= -k_B T \int \exp\left[-\beta\left(\Delta + \frac{(p-p_0)^2}{2\mu_r}\right)\right] \frac{d^3p}{(2\pi\hbar)^3} \\
&= -\frac{4\pi k_B T}{(2\pi\hbar)^3} e^{-\beta\Delta} \int \exp\left[-\beta\frac{(p-p_0)^2}{2\mu_r}\right] p^2 dp \\
&\approx -\frac{4\pi k_B T}{(2\pi\hbar)^3} e^{-\beta\Delta} \int \exp\left[-\beta\frac{(p-p_0)^2}{2\mu_r}\right] p_0^2 dp \\
&\approx -\frac{4\pi k_B T}{(2\pi\hbar)^3} p_0^2 e^{-\beta\Delta} \sqrt{\frac{2\pi\mu_r}{\beta}} \\
&\propto (k_B T)^{3/2} e^{-\Delta/k_B T}.
\end{aligned}$$

In the third line we approximated the factor p^2 in the integral by its value at p_0 since if $p_0 \gg \sqrt{\frac{\mu_r}{\beta}}$, the spread in the gaussian centered at p_0 is very small.