Ben Sauerwine
Practice for Qualifying Exams

Problem Source: **CMU Qualification Exam Day 2 (August 2005)**

The following questions will consider a model material with a density of states given by:

$$D(\varepsilon) = \begin{cases} X & 0 < \varepsilon < A \\ 0 & A \le \varepsilon \le B \\ Y & B < \varepsilon \end{cases}$$

The total number of particles in the system is given by $N = XA$ **for both the Fermi-Dirac and Bose-Einstein parts of the problem.**

Fermi Statistics:

(a) Write the equations for the total energy and number of particles for Fermions.

Let V be the volume of the material.

The grand canonical partition occupation number is given by, for a Fermi gas,

$$Z = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

Now:

$$\langle N\rangle = \int D(\varepsilon)\frac{1}{e^{\beta(\varepsilon-\mu)}+1}d\varepsilon$$

$$\langle E\rangle = \int \varepsilon D(\varepsilon)\frac{1}{e^{\beta(\varepsilon-\mu)}+1}d\varepsilon\,.$$

for

$$\langle N\rangle = \int_0^A X\frac{1}{e^{\beta(\varepsilon-\mu)}+1}d\varepsilon + \int_B^\infty Y\frac{1}{e^{\beta(\varepsilon-\mu)}+1}d\varepsilon$$

$$\langle E\rangle = \int_0^A X\frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}d\varepsilon + \int_B^\infty Y\frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}+1}d\varepsilon$$

(b) **What is the Fermi energy for the limit** $T \to 0$ **?**

The Fermi energy is defined as $\varepsilon_F = \lim_{T\to 0}\mu(T)$. For systems without a band gap, this is the energy of the highest-energy particle in the system in the ground state. For systems with a band gap at the Fermi level, this is in the center of the band gap. Since precisely N particles can be held the lower band in this case, then, the Fermi energy is in the center of the band gap.

Then this energy is $\varepsilon_F = \frac{A+B}{2}$.

(c) Find the chemical potential for low but nonzero temperature.

The chemical potential is chosen so as to keep N constant as temperature increases.

Certainly, then, the chemical potential will lie somewhere between A and B for increasing but low temperatures. Then, I may expand each side in its respective limit as shown below.

Now,

$$N = \int_0^A X \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon + \int_B^\infty Y \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon$$

$$e^{\beta(<A-\mu)} \longrightarrow small$$

$$e^{\beta(>B-\mu)} \longrightarrow big$$

$$\int_0^A X \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \approx \int_0^A X\left(1-e^{\beta(\varepsilon-\mu)}\right) d\varepsilon \quad \int_B^\infty Y \frac{1}{e^{\beta(\varepsilon-\mu)}+1} d\varepsilon \approx \int_B^\infty Y e^{-\beta(\varepsilon-\mu)} d\varepsilon$$

Further,

$$\int_0^A X\left(1-e^{\beta(\varepsilon-\mu)}\right) d\varepsilon = AX - \frac{X}{\beta} e^{\beta(A-\mu)} + \frac{X}{\beta} e^{-\beta\mu} \quad \int_B^\infty Y e^{-\beta(\varepsilon-\mu)} d\varepsilon = \frac{Y}{\beta} e^{-\beta(B-\mu)}$$

Then,

$$N = AX - \frac{X}{\beta} e^{\beta(A-\mu)} + \frac{X}{\beta} e^{-\beta\mu} + \frac{Y}{\beta} e^{-\beta(B-\mu)}$$

$$Xe^{\beta A} e^{-\beta\mu} = Xe^{-\beta\mu} + Ye^{-\beta B} e^{\beta\mu} \quad (use \quad N = AX)$$

$$\ln X + \beta A - \beta\mu = \ln Y - \beta B + \beta\mu \quad \left(neglect \quad Xe^{-\beta\mu}\right)$$

$$\mu(high \quad \beta) \approx \frac{A+B}{2} + \frac{1}{2\beta} \ln \frac{X}{Y}$$

Bose Statistics

(d) Write the equations for the total energy and number of particles for bosons with the given density of states.

Following the procedure from part (a),

$$\langle N\rangle = \int_0^A X\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon + \int_B^\infty Y\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon + N_0$$

$$\langle E\rangle = \int_0^A X\,\frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon + \int_B^\infty Y\,\frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon$$

Recall that due to the singular behavior of Bose-Einstein condensates near $\varepsilon = 0$, I choose to remove this limit and include the number of ‘condensed’ zero-energy particles at zero as N_0.

(e) Describe qualitatively what is meant by Bose-Einstein Condensation

In a Bose-Einstein condensate, a sufficiently high fraction of particles occupies the lowest-energy state that quantum effects become apparent in the macroscopic behavior of the material.

(f) Calculate the temperature at which Bose-Einstein condensation occurs for this density of states.

In particular, the critical temperature for Bose-Einstein condensation occurs where $\mu(T_c) = 0$, as if any additional particles were added they would be forced into the ground state.

Following a procedure similar to part c, then, I have:

$$\langle N\rangle = \int_0^A X\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon + \int_B^\infty Y\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon + N_0$$

However, at low temperatures near T_C, $N_0 \approx 0$. Further, the number of particles in the high-energy band, $\int_B^\infty Y\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon \approx 0$. In fact, there are probably few particles even near the lower end of the band gap, A, so that I can take

$$XA = \langle N\rangle \approx \int_0^A X\,\frac{1}{e^{\beta(\varepsilon-\mu)}-1}\,d\varepsilon = \frac{1}{\beta}\ln\left(\frac{e^{\beta(A-\mu)}-1}{e^{-\beta\mu}-1}\right) - \frac{A}{\beta}$$

$$\beta XA + A = \ln\left(\frac{e^{-\beta\mu}e^{\beta A}-1}{e^{-\beta\mu}-1}\right)$$

Now let me consider the critical temperature where $\mu(\beta_c) = 0$. Here, β_c is large but finite but $\mu(\beta_c) = 0$.

$$\beta_c XA + A = \ln\left(\frac{١e^{\beta_c A} - ١}{١ - ١}\right)$$

Clearly, this diverges and so the only solution is that $\beta_c = \infty$ or $T_c = 0$.

Then, in this material and in fact in any material with a uniform density of states, Bose-Einstein condensation occurs only at absolute zero. In a material in more dimensions, an additional β ٤ dependence would have appeared the density of states which would have made this divergence integrable.