Physics 607

Statistical Physics and Thermodynamics

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Homework #10

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1 Problem #1

(a) For a system where hydrogen penetrates into a solid at a temperature, T, and pressure , P, we assume that within the solid the hydrogen can exist either in the molecular state, H_2 or in the atomic state, H. We can write this as a chemical reaction

$$H_2 \rightarrow 2H$$

We assume that the system satisfies the condition for chemical equilibrium

$$\sum_i \nu_i \mu_i = 0$$

where we only have two different types of chemicals. So we see that $\nu_{H2} = 1$ and $\nu_H = -2$. This implies that

$$\mu_{H2} = 2\mu_H$$

Now we can take the chemical potential for H_2 to be that of an ideal gas

$$\mu_{H2} = T\ln(P) + \chi(T)$$

and assuming that the concentration of atomic hydrogen is small we can take the chemical potential of H to be of the form of a solute

$$\mu_H = T\ln(c) + \psi(P,T)$$

So we can see that if we satisfy the equilibrium condition

$$\begin{aligned}
\mu_{H2} &= 2\mu_H \\
&\Downarrow \\
T\ln(P) + \chi(T) &= 2T\ln(c) + 2\psi(P,T) \\
&\Downarrow \\
\ln(c) &= \frac{1}{2}\ln(P) + \frac{\chi(T) - 2\psi(P,T)}{2T} \\
&\Downarrow \\
c &\propto P^{1/2}
\end{aligned}$$

Note we neglected the ψ dependence on P we have ψ raised a negative exponential which we take to be negligible.

(b) For a reaction of the type

$$AB \rightarrow A + B$$

we can find the concentrations of the components if the reaction starts with the pure AB substance and eventually arrives at the equilibrium state at a fixed temperature and pressure by applying *the law of mass action*

$$\prod_i c_{0i}^{\nu_i} = K_c(P,T) \tag{1.1}$$

Now because we started with pure AB we know that the equilibrium concentrations of the products, A and B, must be the same which yields the condition

$$c_{0A} = c_{0B}$$

Now we also can impose the condition that

$$c_{0AB} + c_{0A} + c_{0B} = 1$$

as we only have those three substances in the system. This combined with our first condition implies

$$c_{0AB} = 1 - 2c_{0A}$$

noting that $\nu_{AB} = 1$ and $\nu_A = \nu_B = -1$ can use equation 1.1 to find

$$c_{0AB}^{1} c_{0A}^{-1} c_{0B}^{-1} = K_c(P,T)$$
$$\Downarrow$$
$$\frac{1 - 2c_{0A}}{c_{0A}^{2}} = K_c(P,T)$$
$$\Downarrow$$
$$1 - 2c_{0A} - K_c(P,T)c_{0A}^{2} = 0$$
$$\Downarrow$$
$$c_{0A} = \frac{\sqrt{K_c(P,T)+1} - 1}{K_c(P,T)} = c_{0B}$$

Note we took the positive solution to the quadratic as we assume that $K_c > 0$ as we increase the concentration of the products. So it follows that

$$c_{0AB} = 1 - 2c_{0A} = \frac{K_c(P,T) - 2\sqrt{K_c(P,T)+1} + 2}{K_c(P,T)}$$

2 Problem #2

(1) We can find the coefficients of the *Bogoliubov transformation* minimizing the ground state energy at zero temperature by noting the transformed Hamiltonian is of the form

$$H_{p,-p} = E^0_{p,-p} + \varepsilon_p \left(\hat{\alpha}^\dagger_p \hat{\alpha}_{-p} + \hat{\alpha}^\dagger_{-p} \hat{\alpha}_p \right)$$

where we take the ground state energy to be

$$E^0_{p,-p} = 2v_p^2 \xi_p - 2gnu_p v_p$$

and

$$\varepsilon_p = \sqrt{\xi_p - (gn)^2}$$

Now we use the condition that $u_p^2 - v_p^2 = 1$ so we can write

$$E^0_{p,-p} = 2v_p^2 \xi_p - 2gn\sqrt{1 + v_p^2}v_p$$

which allows us to calculate the v_p which minimizes $E^0_{p,-p}$ as

$$\frac{\partial E^0_{p,-p}}{\partial v_p} = 0 = 4v_p \xi_p - 2gn\frac{2v_p^2 + 1}{\sqrt{v_p^2 + 1}}$$

$$\Downarrow$$

$$gn\frac{2v_p^2 + 1}{\sqrt{v_p^2 + 1}} = 2v_p \xi_p$$

$$\frac{2v_p^2 + 1}{v_p\sqrt{v_p^2 + 1}} = \frac{2\xi_p}{gn}$$

$$\Downarrow$$

$$\frac{v_p^2(v_p^2 + 1)}{(2v_p^2 + 1)^2} = \frac{\xi_p^2 - \varepsilon_p^2}{4\xi_p^2}$$

$$\Downarrow$$

$$v_p^4 + v_p^2 + \frac{1}{4} = \left(\frac{\xi_p}{2\varepsilon_p} \right)^2$$

$$\Downarrow$$

$$v_p^2 = \frac{1}{2}\left(\frac{\xi_p}{\varepsilon_p} - 1 \right)$$

or if we solve for $u_p^2 = 1 + v_p^2$ we have

$$u_p^2 = \frac{1}{2}\left(\frac{\xi_p}{\varepsilon_p} + 1 \right)$$

Note these are the results we expected as they follow from the transformation derivation.

3 Problem #3

(1) To find the density of the over-condensate particles of a weakly interacting Bose gas at zero temperature by taking the number of particles to be

$$N = N_0 + \sum_{p \neq 0} \hat{a}_p^\dagger \hat{a}_p$$

Where N_0 is the number of particles in the condensate. If we take the *Bogoliubov transformation* where

$$\hat{a}_p = u_p \hat{\alpha}_p - v_p \hat{\alpha}_{-p}^\dagger$$
$$\hat{a}_p^\dagger = -v_p \hat{\alpha}_{-p} + u_p \hat{\alpha}_p^\dagger$$

Which allows us to transform

$$\begin{aligned}
\hat{a}_p^\dagger \hat{a}_p &= \left(-v_p \hat{\alpha}_{-p} + u_p \hat{\alpha}_p^\dagger\right)\left(u_p \hat{\alpha}_p - v_p \hat{\alpha}_{-p}^\dagger\right) \\
&= u_p^2 \hat{\alpha}_p^\dagger \hat{\alpha}_p + v_p^2 \hat{\alpha}_{-p} \hat{\alpha}_{-p}^\dagger - u_p v_p \left(\hat{\alpha}_p^\dagger \hat{\alpha}_{-p}^\dagger + \hat{\alpha}_{-p} \hat{\alpha}_p\right) \\
&= u_p^2 \hat{\alpha}_p^\dagger \hat{\alpha}_p + v_p^2 \left(\hat{\alpha}_{-p}^\dagger \hat{\alpha}_{-p} + 1\right) - u_p v_p \left(\hat{\alpha}_p^\dagger \hat{\alpha}_{-p}^\dagger + \hat{\alpha}_{-p} \hat{\alpha}_p\right) \\
&= v_p^2 + u_p^2 \hat{\alpha}_p^\dagger \hat{\alpha}_p + v_p^2 \hat{\alpha}_{-p}^\dagger \hat{\alpha}_{-p} - u_p v_p \left(\hat{\alpha}_p^\dagger \hat{\alpha}_{-p}^\dagger + \hat{\alpha}_{-p} \hat{\alpha}_p\right) \\
&= v_p^2
\end{aligned}$$

Note that we can neglect all terms that do not conserve momentum which leaves us with the v_p^2 term. Now we evaluate the sum

$$\begin{aligned}
N_e = \sum_{p \neq 0} v_p^2 &= V \int_0^\infty v_p^2 p^2 \frac{d^3 p}{(2\pi\hbar)^3} \\
n_e &= \frac{4\pi}{2(2\pi\hbar)^3} \int_0^\infty p^2 \left(\frac{\xi_p}{\varepsilon_p} - 1\right) dp \\
&= \frac{4\pi}{2(2\pi\hbar)^3} \int_0^\infty p^2 \left(\frac{p^2/2m + gn}{\sqrt{p^2/2m(2gn + p^2/2m)}} - 1\right) dp \\
&= \frac{4\pi 2^{3/2} m^3 s^3}{2(2\pi\hbar)^3} \int_0^\infty y^2 \left(\frac{y^2+1}{\sqrt{x^4 + 2x^2}} - 1\right) dy \\
&= \frac{2^{3/2} m^3 s^3}{2(2\pi\hbar)^3} \frac{\sqrt{2}}{3} \\
&= \frac{4}{3\pi^2} \left(\frac{ms}{\hbar}\right)^3
\end{aligned}$$

Note we used the change of variables

$$s^2 = \frac{gn}{m} \qquad p = (\sqrt{2}ms)x$$

(2) In order to calculate the specific heat of the weakly interacting Bose gas we note that the energy spectrum is given as

$$\varepsilon_p = \sqrt{s^2 p^2 + \left(\frac{p^2}{2m}\right)^2}$$

which we take to the small p limit $\varepsilon_p \approx sp$. This allows us to calculate the energy as

$$\begin{aligned} E &= V \int \frac{\varepsilon_p}{e^{\varepsilon_p/T} - 1} \frac{d^3p}{(2\pi\hbar)^3} \\ &= V \frac{s}{2\pi^2\hbar^3} \int \frac{p^3}{e^{sp/T} - 1} dp \\ &= \frac{V\pi^2 T^4}{30(s\hbar)^3} \end{aligned}$$

Therefore we can find the specific heat as

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{2V\pi^2T^3}{15(s\hbar)^3}$$

and the entropy as

$$S = \frac{E}{T} = \frac{V\pi^2T^3}{30(s\hbar)^3}$$

4 Problem #4

(1) We can find the normal density of the Bogoliubov gas by calculating

$$\begin{aligned}\rho_n &= -\frac{1}{3}\int p^2 \frac{df}{d\varepsilon_p}\frac{d^3p}{(2\pi\hbar)^3} \\ &= \frac{1}{3}\frac{1}{2\pi^2\hbar^3}\int p^4 \frac{e^{sp/T}}{e^{sp/T}-1}dp \\ &= \frac{4\zeta(5)T^5}{\pi^2\hbar^3 s^5}\end{aligned}$$

and the superfluid density as

$$\begin{aligned}\rho_s &= -\frac{1}{3s}\int p^2 \frac{df}{dp}\frac{d^3p}{(2\pi\hbar)^3} \\ &= \frac{1}{3}\frac{1}{2\pi^2\hbar^3}\frac{1}{T}\int p^4 \frac{e^{sp/T}}{(e^{sp/T}-1)^2}dp \\ &= \frac{2\pi T^4}{45\hbar^3 s^5}\end{aligned}$$

We note the difference in the power of T this results in the limited case where $T >> gn = ms^2$ it will result in a normal density that goes to one and a super fluid density that goes to zero. In the other limit we see that both densities becomes smaller than one.

(2) We can compare the results for the condensate density found as

$$\begin{aligned}n &= \int \frac{1}{e^{\varepsilon_p/T}-1}\frac{d^3p}{(2\pi\hbar)^3} \\ &= \frac{1}{2\pi^2\hbar^3}\int \frac{p^2}{e^{sp/T}-1}dp \\ &= \frac{2\zeta(3)T^3}{2\pi^2(s\hbar)^3}\end{aligned}$$

we see that this differs from the normal density by a factor of $(T/s)^2$.