INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2010

Answers to Questions III. Oct. 11th.

Here is an outline of the solutions.

1. (a) We begin by writing down the partition function

$$Z = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu N)}\right] \tag{1}$$

Differentiating w.r.t. μ, we have

$$\frac{\partial Z}{\partial \mu} = \beta \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu N)}\hat{N}\right] \tag{2}$$

So putting $F = (-1/\beta)\mathrm{ln}Z$, we have

$$-\frac{\partial F}{\partial \mu} = \frac{1}{\beta Z}\frac{\partial Z}{\partial \mu} = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu N)}\hat{N}\right] = \langle \hat{N} \rangle \tag{3}$$

(b) If we take

$$H - \mu N = (\epsilon - \mu)a^\dagger a \tag{4}$$

then the partition function is

$$Z = \begin{cases} \sum_{n=0}^{\infty} e^{-\beta n(\epsilon-\mu)} = (1 - e^{-\beta(\epsilon-\mu)})^{-1} & \text{(Boson)} \\ 1 + e^{-\beta(\epsilon-\mu)} & \text{(Fermion)} \end{cases} \tag{5}$$

Taking the logarithm of these expressions, we obtain

$$F = -k_B T \mathrm{ln} Z = \pm k_B T \mathrm{ln}[1 \mp e^{-\beta(\epsilon-\mu)}] \tag{6}$$

where the upper sign refers to bosons, the lower, to fermions. Finally, taking the derivative of this expression w.r.t. μ yields

$$-\frac{\partial F}{\partial \mu} = \langle \hat{n} \rangle = \frac{1}{e^{\beta(\epsilon-\mu)} \mp 1} \tag{7}$$

2. (a) We may estimate the Bose Einstein transition temperature from

$$T_{BE} = \frac{3.31}{k_B}\left(\frac{\hbar^2 n^{2/3}}{m}\right) = \frac{3.31}{1.38 \times 10^{-23}}\left(\frac{\hbar^2 (10^{21} m^{-3})^{2/3}}{23 m_p}\right) \approx 6.9 \mu K.$$

These tiny temperatures are attained by "evaporative cooling" . Sodium atoms are held in a "magneto-optic" trap. Radio waves are used to "evaporate" the most energetic atoms in the trap, leaving behind the cold ones.

(b) In Helium-4, we may estimate the Bose Einstein transition temperature as

$$T_{BE} = \frac{3.31}{k_B}\left(\frac{\hbar^2 n^{2/3}}{m_{He}}\right) = \frac{3.31}{1.38\times 10^{-23}}\left(\frac{\hbar^2((122/(4m_p)))^{2/3}}{4m_p}\right) \approx 2.76K.$$

The actual condensation temperature is 2.21K. The difference in condensation temperatures is due to the repulsive interaction between atoms.

(a) If the interaction has the form

$$V(r) = \begin{cases} U, & (r < R), \\ 0, & (r > R), \end{cases} \tag{8}$$

then in second-quantized form, the interaction Hamiltonian is

$$V = \frac{U}{2}\sum_{\sigma,\sigma'}\int d^3x \int_{|\vec{x}'-\vec{x}|<R} d^3x' [\psi^\dagger{}_\sigma(x)\psi^\dagger{}_{\sigma'}(x')\psi_{\sigma'}(x')\psi_\sigma(x)]. \tag{9}$$

(ii) Inverting the Fourier transform, we have $c_{\vec{k}\sigma} = \int d^3x\psi_\sigma(\vec{x})e^{-i\vec{k}\cdot\vec{x}}$, so that

$$\begin{aligned} [c_{\vec{k}\sigma},\ c^\dagger{}_{\vec{k}'\sigma'}]_\pm &= \int d^3x d^3x' [\psi_\sigma(x),\ \psi^\dagger{}_{\sigma'}(x')]_\pm e^{-i(\vec{k}\cdot\vec{x}-\vec{k}'\cdot\vec{x}')} \\ &= \delta_{\sigma\ \sigma'}\int d^3x e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}} \\ &= \delta_{\sigma\ \sigma'}(2\pi)^3\delta^{(3)}(\vec{k}-\vec{k}'). \end{aligned} \tag{10}$$

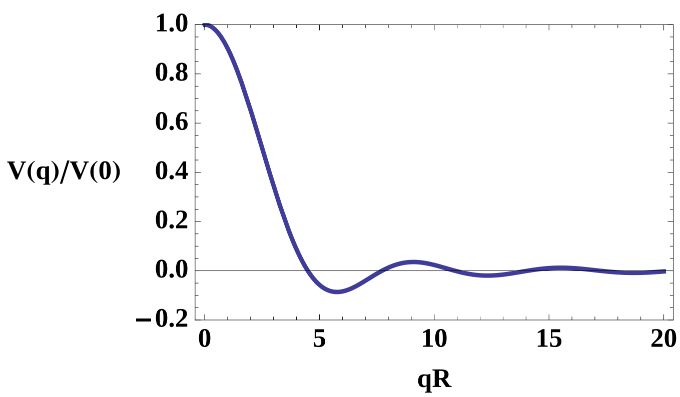

Figure 1: Fourier transformed potential $V(q)$ for "hard sphere" potential.

(iii) In momentum space, we may write

$$V = \frac{1}{2}\int \frac{d^3k d^3k' d^3q}{(2\pi)^9} V(q)\left[c^\dagger{}_{\vec{k}+\vec{q}\sigma}c^\dagger{}_{\vec{k}'-\vec{q}\sigma'}c_{\vec{k}'\sigma'}c^\dagger{}_{\vec{k}\sigma}\right], \tag{11}$$

where

$$V(\vec{q}) = \int d^3x V(\vec{x})e^{i\vec{q}\cdot\vec{x}} = \frac{4\pi U}{q}\int_0^R dr r\sin(qr) = \left(\frac{4\pi R^3 U}{3}\right)F(qR) \tag{12}$$

and

$$F(x) = \frac{3}{x^2}\left[\frac{\sin x}{x} - \cos x\right]. \tag{13}$$

The form of the interaction in momentum space is sketched above. The hard core in real space is manifested as a long-range oscillatory component in momentum space.

3. Let us start with the density of states for the microcanonical ensemble,

$$W(E,N) = \mathrm{Tr}\left[\delta(E-\hat{H})\delta(N-\hat{N})\right]$$

where N and E are the particle number and energy of states in the ensemble, respectively.

(a) Writing the delta functions as Fourier transforms (inverse Laplace transforms, we obtain

$$\begin{aligned} W(E,N) &= \int_{\beta_0-i\infty}^{\beta_0+i\infty}\int_{\zeta_0-i\infty}^{\zeta+i\infty}\frac{d\beta d\zeta}{(2\pi i)^2}\mathrm{Tr}\left[e^{\beta(E-\hat{H})+\zeta(N-\hat{N})}\right] \\ &= \int_{\beta_0-i\infty}^{\beta_0+i\infty}\int_{\zeta_0-i\infty}^{\zeta_0+i\infty}\frac{d\beta d\zeta}{(2\pi i)^2}e^{\beta E-\zeta N}\overbrace{\mathrm{Tr}\left[e^{-\beta\hat{H}+\zeta\hat{N}}\right]}^{\tilde{Z}[\beta,\zeta]} \\ &= \int_{\beta_0-i\infty}^{\beta_0+i\infty}\int_{\zeta_0-i\infty}^{\zeta_0+i\infty}\frac{d\beta d\zeta}{(2\pi i)^2}e^{\beta E-\zeta N+\ln\tilde{Z}[\beta,\zeta]} \end{aligned} \tag{14}$$

Making the identification $\zeta = \mu\beta$, we recognize

$$\tilde{Z}[\beta,\zeta] \equiv Z[\beta,\mu] = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]$$

as the partition function of the Grand Canonical ensemble.
Now in a large system, we can approximate this integral by the value of the integrand at the stationary point,

$$W \approx e^{\beta_0(E-\mu_0 N)+\ln Z[\beta_0,\mu_0]}, \tag{15}$$

where β_0 and $\zeta_0 = \mu_0\beta_0$ are determined by the stationarity conditions

$$\frac{\partial(\beta E-\zeta N+\ln\tilde{Z})}{\partial\beta} = E + \frac{\partial\ln\tilde{Z}}{\partial\beta} = 0 \tag{16}$$

or $E = -\frac{\partial\ln\tilde{Z}}{\partial\beta}$ and

$$\frac{\partial(\beta E-\zeta N+\ln\tilde{Z})}{\partial\zeta} = -N + \frac{\partial\ln\tilde{Z}}{\partial\zeta} = 0 \tag{17}$$

or

$$E_0 = -\frac{\partial(\ln\tilde{Z})}{\partial\beta}, \qquad N = -\frac{\partial(-\beta^{-1}\ln\tilde{Z})}{\partial\mu}, \tag{18}$$

where we have dropped the subscripts "0" from β and ζ. From thermodynamics, we know that if F is the Free energy, $dF = -SdT - Nd\mu$ and that $F = E - TS - \mu N$, so that $d(F\beta) = Ed\beta - d(\mu\beta)N = Ed\beta - d\zeta N$, i.e $\partial(F\beta)/\partial\beta = E$, $\partial(F\beta)/\partial\zeta = -N$. Comparing these relations with (16) and (17), we can identify $\beta F = -\ln Z$, i.e $-\beta^{-1}\ln Z = E - TS - \mu N$ is the Free energy, thus from (15)

$$\ln W = \beta(E - \mu N) - \beta F.$$

But since $F = E - TS - \mu N$, it follows that

$$\ln W = \beta(E - \mu N) - \beta(E - TS - \mu N) = \frac{1}{k_B} S,$$

the entropy, so that

$$S[E, N] = k_B \ln W.$$

(b) The equivalence between the Grand and microcanonical ensembles holds for quantities that are coarse-grained functions of the particle number and energy. Let us suppose that $\hat{A} = A(\hat{H}, \hat{N})$ is a slowly varying function of particle number and energy. The passage from the micro- to the Grand canonical ensemble is made by coarse-graining the delta functions inside the density matrix. Let us see how this works here. Replacing the delta functions by integrals, we obtain

$$\begin{aligned} \langle \hat{A} \rangle_M &= \frac{1}{W} \mathrm{Tr}[\hat{A}\delta(E - \hat{H})\delta(N - \hat{N})] \\ &= \frac{1}{W} \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \int_{\zeta - i\infty}^{\zeta_0 + i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} \mathrm{Tr}\left[\hat{A}\ e^{\beta(E_0 - \hat{H}) + \zeta(N - \hat{N})}\right]. \end{aligned} \tag{19}$$

Now provided $\hat{A}$ commutes with $\hat{N}$ and $\hat{H}$, we may rewrite this expression as a derivative w.r.to a source term,

$$\begin{aligned} \langle \hat{A} \rangle_M &= \frac{1}{W} \frac{\partial}{\partial \lambda} \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} \mathrm{Tr}\left[\ e^{\beta(E - \hat{H}) + \zeta(N - \hat{N}) + \lambda \hat{A}}\right]\Bigg|_{\lambda = 0} \\ &= \frac{\partial \ln W[E, N, \lambda]}{\partial \lambda} \end{aligned} \tag{20}$$

where

$$W = \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} \mathrm{Tr}\left[\ e^{\beta(E - \hat{H}) + \zeta(N - \hat{N}) + \lambda \hat{A}}\right]$$

Carrying out this last integral by saddle-point techniques, we obtain

$$\begin{aligned} W[E, N, \lambda] &= e^{\beta_0 E - \zeta_0 N} \tilde{Z}[\beta_0, \zeta, \lambda] \\ &= e^{\beta_0 (E - \mu_0 N)} \tilde{Z}[\beta_0, \mu, \lambda] = \end{aligned} \tag{21}$$

where now

$$\tilde{Z}[\beta, \zeta, \lambda] = Z[\beta, \mu, \lambda] = \mathrm{Tr}\left[\ e^{-\beta(\hat{H} - \mu \hat{N}) + \lambda \hat{A}}\right]$$

subject to the conditions that $E_0 = -\partial \ln \tilde{Z}/\partial \beta$ and $N_0 = \partial \ln Z/\partial \mu$. Taking the logarithmic derivative of both sides, we then obtain

$$\langle A \rangle_M = \frac{1}{Z} \mathrm{Tr}\left[\hat{A}\ e^{-\beta(\hat{H} - \mu \hat{N}) + \lambda \hat{A}}\right] = \langle A \rangle_G$$