INTRODUCTION TO MANY BODY PHYSICS: 620. Fall 2015

Answers to Questions III. Oct. 16th

Here is an outline of the solutions.

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

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

(1)

Differentiating w.r.t. \( \mu \), we have

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

(2)

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

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

(3)

(b) If we take

\[ H - \mu \hat{N} = (\epsilon - \mu) \hat{a}^\dagger \hat{a} \]  

(4)

then the partition function is

\[ Z = \left\{ \sum_{n=0}^{\infty} e^{-\beta n(\epsilon - \mu)} = \begin{cases} 1 - e^{-\beta (\epsilon - \mu)}^{-1} & \text{(Boson)} \\ 1 + e^{-\beta (\epsilon - \mu)} & \text{(Fermion)} \end{cases} \right. \]  

(5)

Taking the logarithm of these expressions, we obtain

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

(6)

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

\[ -\frac{\partial F}{\partial \mu} = \langle \hat{n} \rangle = \frac{1}{e^{\beta (\epsilon - \mu)} + 1} \]  

(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.
Figure 1: Occupancies $n(\epsilon)$ and $f(\epsilon)$ for a range of temperatures.

(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.

3. (a) If the interaction has the form

$$V(r) = \begin{cases} U, & (r < R), \\ 0, & (r > R), \end{cases}$$  \hspace{1cm} (8)

then in second-quantized form, the interaction Hamiltonian is

$$V = \frac{U}{2} \sum_{\sigma, \sigma'} \int d^3x \int_{|\vec{x}' - \vec{x}| < R} d^3x' \left[ \psi^\dagger_\sigma(x) \psi^\dagger_{\sigma'}(x') \psi_{\sigma'}(x') \psi_\sigma(x) \right].$$ \hspace{1cm} (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

$$[c_{\vec{k} \sigma}, c^\dagger_{\vec{k}' \sigma'}]_\pm = \int d^3x d^3x' \left[ \psi_\sigma(x), \psi^\dagger_{\sigma'}(x') \right]_\pm e^{-i(\vec{k} - \vec{k}') \cdot \vec{x}}$$

$$= \delta_{\sigma \sigma'} \delta_{ \pm } \int d^3x e^{-i(\vec{k} - \vec{k}') \cdot \vec{x}}$$

$$= \delta_{\sigma \sigma'} (2\pi)^3 \delta^{(3)}(\vec{k} - \vec{k}').$$ \hspace{1cm} (10)

(iii) In momentum space, we may write

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

where

$$V(q) = \int d^3x V(\vec{x}) e^{i\vec{q} \cdot \vec{x}} = \frac{4\pi U}{q} \int_0^R dr r \sin(qr) = \left( \frac{4\pi R^3 U}{3} \right) F(qR)$$ \hspace{1cm} (12)
Figure 2: Fourier transformed potential $V(q)$ for “hard sphere” potential.

and

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

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.

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

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

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

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

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

$$= \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} e^{\beta E - \zeta N + \ln Z[\beta, \zeta]} \quad (14)$$

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

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

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,

$$W \approx e^{\beta_0 (E - \mu_0 N) + \ln Z[\beta_0, \mu_0]}, \quad (15)$$
where $\beta_0$ and $\zeta_0 = \mu_0 \beta_0$ are determined by the stationarity conditions
\[
\frac{\partial (\beta E - \zeta N + \ln Z)}{\partial \beta} = E + \frac{\partial \ln \tilde{Z}}{\partial \beta} = 0
\] (16)
or $E = -\frac{\partial \ln \tilde{Z}}{\partial \beta}$ and
\[
\frac{\partial (\beta E - \zeta N + \ln Z)}{\partial \zeta} = -N + \frac{\partial \ln \tilde{Z}}{\partial \zeta} = 0
\] (17)
or
\[
E_0 = -\frac{\partial (\ln \tilde{Z})}{\partial \beta}, \quad N = -\frac{\partial (-\beta^{-1} \ln \tilde{Z})}{\partial \mu},
\] (18)
where we have dropped the subscripts “0” from $\beta$ and $\zeta$. From thermodynamics, we know that if $F$ is the Free energy, $dF = -SdT - N d\mu$ 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 $\hat{A} = \hat{A}(\hat{H}, \hat{N})$ 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
\[
\langle \hat{A} \rangle_M = \frac{1}{W} \text{Tr} \left( \hat{A} \delta(E - \hat{H}) \delta(N - \hat{N}) \right) = \frac{1}{W} \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} \text{Tr} \left( \hat{A} e^{\beta(E_0 - \hat{H}) + \zeta(N - \hat{N})} \right) \bigg|_{\lambda = 0}.
\] (19)
Now using the result $\frac{\partial}{\partial \lambda} \text{Tr} \left( e^{\lambda A + B} \right) = \text{Tr} \left( A e^{\lambda A + B} \right)$, (which you may verify by expanding the exponential as a power series, holds even if $\hat{A}$ and $\hat{B}$ do not commute), we can rewrite this expression as a derivative w.r. to a source term,
\[
\langle \hat{A} \rangle_M = \frac{\partial}{\partial \lambda} \frac{1}{W} \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} \int_{\zeta_0 - i\infty}^{\zeta_0 + i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} \text{Tr} \left( e^{\beta(E - \hat{H}) + \zeta(N - \hat{N}) + \lambda \hat{A}} \right) \bigg|_{\lambda = 0}.
\] (20)
where
\[
W = \int_{\beta_0-i\infty}^{\beta_0+i\infty} \int_{\zeta_0-i\infty}^{\zeta_0+i\infty} \frac{d\beta d\zeta}{(2\pi i)^2} \text{Tr} \left[ e^{\beta(E-H)+\zeta(N-\mathcal{N})+\lambda\mathcal{A}} \right]
\]

Carrying out this last integral by saddle-point techniques, we obtain
\[
W[E,N,\lambda] = e^{\beta_0 E - \zeta_0 N} \tilde{Z}[\beta_0,\zeta,\lambda] = \frac{\tilde{Z}[\beta_0,\mu,\lambda]}{\tilde{Z}[\beta_0,\zeta,\lambda]} = e^{\beta_0 (E-\mu N)} \tilde{Z}[\beta_0,\mu,\lambda] = (21)
\]

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

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