Physics 413: Stat. Mech. - Solutions of Homework 5

Problem 1: Relativistic ideal gas

a) eigenstates are plane waves $\psi_{\mathbf{k}} = V^{-1/2} e^{i\mathbf{k}\cdot\mathbf{x}}$ with wavevectors $k_i = (2\pi/L)n_i$ with n_i integer
$\epsilon = c|\mathbf{p}| = c\hbar\,\sqrt{k_x^2 + k_y^2 + k_z^2}$
Total energy

$$E = c\hbar \sum_{i=1}^{N} \sqrt{(k_{i,x}^2 + k_{i,y}^2 + k_{i,z}^2)}$$

To count microstates we need the volume of the object defined by this equation in $3N$-dimensional $\mathbf{k}$-space. The length scale of the object is $R_{\mathbf{k}} = E/(c\hbar)$. Thus, the volume is $V_{\mathbf{k}} = B(N)\,[E/(c\hbar)]^{3N}$ where the constant prefactor only depends on N.

The number of states with energies below E, is therefore

$$\Sigma(E,N,V) = V_{\mathbf{k}}/(2\pi/L)^{3N} = B(N)\left(\frac{LE}{ch}\right)^{3N}$$

$$\Omega(E,N,V) \sim \partial\Sigma(E,N,V)/\partial E \sim \frac{3N}{E}\Sigma(E,N,V)$$

In calculating S we use the fact that it has to be extensive to pull the appropriate factors of N into the logarithm:

$$S(E,N,V) = Nk_B \ln\left[\frac{V}{N}\left(\frac{E}{Nch}\right)^3\right] + f(N)$$

b) Solve for the energy:

$$E = Nch(N/V)^{1/3} e^{\frac{S-f(N)}{3Nk_B}}$$

temperature $T = (\partial E/\partial S)_{N,V} = E/(3Nk_BT)$, therefore $E = 3Nk_BT$.

c) pressure $T = -(\partial E/\partial V)_{N,S} = E/(3V) = Nk_BT/V$, therefore $pV = Nk_BT$.

d) $C_p - C_v = TV\alpha^2/\kappa_T$
The r.h.s. only depends on the thermodynamic eq. of state, thus it is the same as for the non-relativistic ideal gas: $C_p - C_v = Nk_B$
Therefore: $C_p = 4Nk_B$ and $C_p/C_v = 4/3$.

Problem 2: Comparison of the microcanonical and canonical ensembles: system of two-level atoms

a) Microcanonical ensemble

$N_0 + N_1 = N$, $n_0 = N_0/N$, $n_1 = N_1/N$, $n_0 + n_1 = 1$, $E = N_0E_0 + N_1E_1 = N_1\epsilon$

(i) $\Omega = N!/(N_0!N_1!)$
$S = k_B \ln \Omega = k_B[\ln(N!) - \ln(N_0!) - \ln(N_1!)]$
minimum S: $S = 0$ for $N_0 = 0, N_1 = N$ or $N_0 = N, N_1 = 0$
(just a single microstate, i.e maximum order)
maximum S: $S = k_B[\ln(N!) - 2\ln(N/2!)]$
(maximum disorder)
$S/N = (k_B/N)[N \ln N - N - N_0 \ln N_0 + N_0 - N_1 \ln N_1 + N_1]$
$S/N = k_B[-(N_0/N) \ln N_0 - (N_1/N) \ln N_1 + \ln N]$
$S/N = k_B[-(N_0/N) \ln(N_0/N) - (N_1/N) \ln(N_1/N)]$
$S/N = k_B[-n_0 \ln n_0 - n_1 \ln n_1]$

(ii) $1/T = (\partial S/\partial E)$, $E = N_1\epsilon$
$1/T = (1/\epsilon)(\partial S/\partial N_1) = (1/\epsilon)(\partial(S/N)/\partial(N_1/N))$
$1/T = (k_B/\epsilon)(\partial/\partial n_1)[-(1 - n_1) \ln(1 - n_1) - n_1 \ln n_1]$
$1/T = (k_B/\epsilon)[\ln(1 - n_1) + 1 - \ln n_1 - 1]$
$1/T = (k_B/\epsilon) \ln(n_0/n_1)$
$k_B T = \epsilon/ \ln(n_0/n_1)$
$T > 0$ if $n_0 > n_1$, usual case – occupation probability decreases with increasing energy
$T < 0$ if $n_0 < n_1$, inversion, important i.e in lasers, in *equilibrium* only possible with bounded energy spectrum
with increasing energy the temperature goes $T = 0+ \to +\infty \to -\infty \to 0-$

(iii) $C = (\partial E/\partial T) = \epsilon(\partial N_1/\partial T)$
$1/C = (1/\epsilon)(\partial T/\partial N_1) = 1/(Nk_B)(\partial/\partial n_1)[1/ \ln((1 - n_1)/n_1)]$
$1/C = -1/(Nk_B)1/ \ln^2(n_0/n_1)(-1/n_0 - 1/n_1)$
$C = Nk_B n_0 n_1 \ln^2(n_0/n_1)$ $\quad$ $C > 0$ for all temperatures!

b) (i)

$$Z_1(\beta) = 1 + e^{-\beta\epsilon}, \quad p_0 = 1/(1 + e^{-\beta\epsilon}), \quad p_1 = e^{-\beta\epsilon}/(1 + e^{-\beta\epsilon})$$
$$A = -Nk_B T \ln Z_1(\beta) = -Nk_B T \ln(1 + e^{-\beta\epsilon})$$

(ii)

$$U = -N(\partial \ln Z_1/\partial\beta) = N\epsilon e^{-\beta\epsilon}/(1 + e^{-\beta\epsilon}) = N\epsilon p_1$$
$$TS = (U - A) = N\epsilon e^{-\beta\epsilon}/(1 + e^{-\beta\epsilon}) + Nk_B T \ln(1 + e^{-\beta\epsilon})$$
$$C = (\partial U/\partial T) = \frac{N\epsilon^2}{k_B T^2} \frac{e^{\epsilon/k_B T}}{(1 + e^{\epsilon/k_B T})^2}$$

(iii)

$$k_B T = \epsilon/ \ln(p_0/p_1)$$
$$U = N\epsilon p_1$$
$$C = Nk_B \ln^2(p_0/p_1)p_0 p_1$$
$$S = -k_B(p_0 \ln p_0 + p_1 \ln p_1)$$

Results are identical to those obtained from the microcanonical approach above.

Problem 3: Two interacting magnetic moments

a) In the ground state, the two moments will be parallel.

b)

$$Q = \int d\phi d\theta \ \sin\theta \ \exp(\beta J \cos\theta) = 2\pi \int_{-1}^{1} dx \ \exp(\beta J x) = \frac{4\pi}{\beta J}\sinh(\beta J)$$

$$A = -k_B T \ln\left[\frac{4\pi}{\beta J}\sinh(\beta J)\right]$$

c)

$$\langle E\rangle = -\frac{\partial \ln Q}{\partial \beta} = -J\coth(\beta J) + 1/\beta$$

$$C = \frac{\partial\langle E\rangle}{\partial T} = k_B\left[1 + \frac{J^2}{k_B^2 T^2}(1 - \coth^2(\beta J))\right]$$

d) At low temperatures, the angle θ will be small. Thus we can expand $\sin\theta \approx \theta$ and $\cos\theta \approx 1 - \theta^2/2$.

$$\langle\theta\rangle = \frac{\int_0^\infty \theta d\theta \ \theta \exp(-\beta J\theta^2/2)}{\int_0^\infty \theta d\theta \ \exp(-\beta J\theta^2/2)} = \sqrt{\pi/(2\beta J)}$$

$$\langle\theta^2\rangle = \frac{\int_0^\infty \theta d\theta \ \theta^2 \exp(-\beta J\theta^2/2)}{\int_0^\infty \theta d\theta \ \exp(-\beta J\theta^2/2)} = 2/(\beta J)$$

$$\langle\theta^2\rangle - \langle\theta\rangle^2 = \frac{k_B T}{J}(2 - \pi/2)$$

One could argue that $\langle\theta\rangle = 0$ because of symmetry. This depends on how exactly you define θ. I count both answers as correct.