

Model Solutions for First Exam

1. Heat capacity

The Sackur-Tetrode formula is

$$S(E, V, N) = k_B N \left[\frac{3}{2} \ln \left(\frac{4\pi m E V^{2/3}}{3h_0^2 N^{5/3}} \right) + \frac{5}{2} \right]. \quad (1)$$

Use $E = \frac{3}{2} N k_B T$ to write

$$S(T, V, N) = k_B N \left[\frac{3}{2} \ln \left(\frac{2\pi m k_B T V^{2/3}}{h_0^2 N^{5/3}} \right) + \frac{5}{2} \right], \quad (2)$$

then find

$$C_V(T, V, N) = T \left(\frac{\partial S}{\partial T} \right)_{V, N} = \frac{3}{2} k_B N.$$

Use $V = N k_B T / p$ in equation (2) to write

$$S(T, p, N) = k_B N \left[\frac{3}{2} \ln \left(\frac{2\pi m (k_B T)^{5/3}}{h_0^2 p^{2/3}} \right) + \frac{5}{2} \right], \quad (3)$$

then find

$$C_p(T, p, N) = T \left(\frac{\partial S}{\partial T} \right)_{p, N} = \frac{5}{2} k_B N.$$

2. The coin toss

A single coin is tossed seven times.

- The probability of obtaining all heads is $1/2^7$.
- The probability of obtaining alternating heads and tails is $2/2^7$. (One alternating pattern starts with heads, the other starts with tails.)
- The probability of obtaining the pattern THHTHTT is $1/2^7$.
- The probability of obtaining a pattern with one head and six tails is $7/2^7$. (There are seven such patterns.)

3. Thermodynamics of a new substance

The entropy of a newly discovered gas is determined to be

$$S(E, V, N) = \left(\frac{k_B}{T_0} \right)^{1/2} \left[N E + \frac{k_B T_0 V^2}{v_0^2} \right]^{1/2},$$

where the constants T_0 and v_0 are positive, intensive quantities with the dimensions of temperature and volume, respectively.

- a. *Extensivity*: NE goes up like N^2 , and V^2 goes up like N^2 , so the stuff in square brackets goes up like N^2 . Thus square root goes up like N , but the stuff in parentheses is independent of N , so S is extensive, as required.

Dimensions: NE has the dimensions of energy and $k_B T_0 V^2 / v_0^2$ has the dimensions of energy, so the stuff in square brackets has the dimensions of energy and the square root has dimensions [energy]^{1/2}. Thus the expression for S has the dimensions of

$$\left(\frac{k_B E}{T}\right)^{1/2} = \left(\frac{k_B T E}{T^2}\right)^{1/2} = \left(\frac{E^2}{T^2}\right)^{1/2} = \frac{E}{T}$$

and these are the dimensions of entropy.

- b. We are to find $T(S, V, N)$ and $p(S, V, N)$, so we first invert the function to find $E(S, V, N)$. Straightforward algebra gives

$$E(S, V, N) = \frac{T_0}{k_B} \frac{S^2}{N} - \frac{k_B T_0}{v_0^2} \frac{V^2}{N}.$$

Then

$$T(S, V, N) = \left(\frac{\partial E}{\partial S}\right)_{V, N} = 2 \frac{T_0}{k_B} \frac{S}{N}$$

and

$$p(S, V, N) = - \left(\frac{\partial E}{\partial V}\right)_{S, N} = 2 \frac{k_B T_0}{v_0^2} \frac{V}{N}.$$

Note: If you didn't read the problem carefully and instead found $T(E, V, N)$ and $p(E, V, N)$ then, with considerably more difficulty, you found

$$T(E, V, N) = \left[\frac{\partial S}{\partial E}\right]_{V, N}^{-1} = 2 \left(\frac{k_B}{T_0}\right)^{1/2} \left[\frac{E}{N} + \frac{k_B T_0}{v_0^2} \left(\frac{V}{N}\right)^2\right]^{1/2}$$

and

$$p(E, V, N) = T(E, V, N) \left(\frac{\partial S}{\partial V}\right)_{E, N} = 2 \frac{k_B T_0}{v_0^2} \frac{V}{N}.$$

4. Accessible configurations in another spin system

In this system the energy resides not in the *spins*, but in the nearest-neighbor *pairs* (sometimes called the *bonds*). The spins can be up (U) or down (D) — the pairs can be alike (A) or different (D). The spin configuration UUDU has a pair configuration ADD. (There are two spin configurations for each pair configuration: one starting with an up spin and the other starting with a down spin.) Thus the problem becomes very similar to the ideal paramagnet, but instead of N high- or low-energy *spins*, we have $N - 1$ high- or low-energy *pairs*.

- a. Maximum possible energy (all pairs alike — spins either all up or all down): $-(N - 1)J$.
 Minimum possible energy (all pairs different — spins alternate up and down): $+(N - 1)J$.
 Smallest possible energy spacing between configurations: $2J$.

- b. The energy of a configuration depends only on the number of alike pairs n_A and the number of different pairs n_D :

$$E = -Jn_A + Jn_D \quad \text{where} \quad N - 1 = n_A + n_D. \quad (4)$$

In a parallel to the poker hand problem, the number of configurations with exactly this energy is

$$2 \frac{(N-1)!}{n_A!n_D!}.$$

Solving equations (4) for n_A and n_D in terms of E and N gives

$$n_A = \frac{1}{2}((N-1) - E/J) \quad \text{and} \quad n_D = \frac{1}{2}((N-1) + E/J).$$

Finally, the number of permissible energies within energy range ΔE is $\Delta E/(2J)$, so the approximate number of configurations with energy between E and $E + \Delta E$ is

$$\Omega(E, \Delta E, J, N) = \frac{(N-1)!}{n_A!n_D!} \left(\frac{\Delta E}{J} \right)$$

where

$$n_A = \frac{1}{2}((N-1) - E/J) \quad \text{and} \quad n_D = \frac{1}{2}((N-1) + E/J).$$

- c.

$$\begin{aligned} S(E, \Delta E, J, N)/k_B &= \ln((N-1)!) - \ln(n_A!) - \ln(n_D!) + \ln(\Delta E/J) \\ &= \ln((N-1)!) - \ln([\tfrac{1}{2}((N-1) - E/J)]!) - \ln([\tfrac{1}{2}((N-1) + E/J)]!) + \ln(\Delta E/J) \end{aligned}$$

- d. Define

$$e = \frac{E}{N-1},$$

so that

$$n_A = \frac{1}{2}(1 - e/J)(N-1) \quad \text{and} \quad n_D = \frac{1}{2}(1 + e/J)(N-1).$$

Then Stirling's approximation tells us that

$$\begin{aligned} &\ln((N-1)!) - \ln(n_A!) - \ln(n_D!) \\ &\approx (N-1)\ln(N-1) - (N-1) - n_A \ln(n_A) + n_A - n_D \ln(n_D) + n_D \\ &= (N-1)\ln(N-1) - n_A \ln(n_A) - n_D \ln(n_D) \\ &= (N-1)\ln(N-1) - n_A \ln(\tfrac{1}{2}(1 - e/J)(N-1)) - n_D \ln(\tfrac{1}{2}(1 + e/J)(N-1)) \\ &= (N-1)\ln(N-1) - n_A \ln(\tfrac{1}{2}(1 - e/J)) - n_A \ln(N-1) - n_D \ln(\tfrac{1}{2}(1 + e/J)) - n_D \ln(N-1) \\ &= -n_A \ln(\tfrac{1}{2}(1 - e/J)) - n_D \ln(\tfrac{1}{2}(1 + e/J)) \\ &= -\tfrac{1}{2}(1 - e/J)(N-1) \ln(\tfrac{1}{2}(1 - e/J)) - \tfrac{1}{2}(1 + e/J)(N-1) \ln(\tfrac{1}{2}(1 + e/J)). \end{aligned}$$

We are interested in the thermodynamic limit ($N \rightarrow \infty$) of the expression

$$\frac{S(E, \Delta E, J, N)}{k_B N} = \frac{\ln((N-1)!) - \ln(n_A!) - \ln(n_D!)}{N} + \frac{\ln(\Delta E/J)}{N}.$$

The rightmost part is easy: it vanishes like $\ln(N)/N$ as $N \rightarrow \infty$. Putting these pieces together, we find that the thermodynamic limit of $S(E, \Delta E, J, N)/k_B N$ is

$$\begin{aligned} s(e, J)/k_B &= -\frac{1}{2}(1 - e/J) \ln\left(\frac{1}{2}(1 - e/J)\right) - \frac{1}{2}(1 + e/J) \ln\left(\frac{1}{2}(1 + e/J)\right) \\ &= -\frac{1}{2}(1 - e/J) \ln(1 - e/J) - \frac{1}{2}(1 + e/J) \ln(1 + e/J) + \ln(2). \end{aligned}$$