PY541 PS5

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Problem 1:
Two Magnetic Systems in Thermal Contact (Gould 4.38)

Before getting to the problem, making the following table will be useful. The total number of microstates is

E_A	E_B	$\uparrow\downarrow A$	$\uparrow\downarrow$ B	$\Omega(E_A)$	$\Omega(E_B)$	$\Omega(E_A)\Omega(E_B)$	$P_A(E_A)$
-4μB	0 μB	$\uparrow \times 4 \downarrow \times 0$	$\uparrow \times 8 \downarrow \times 8$	1	12870	12870	0.1022
-2μB	-2μB	$\uparrow \times 3 \downarrow \times 1$	$\uparrow \times 9 \downarrow \times 7$	4	11440	45760	0.3633
0μB	-4μB	$\uparrow \times 2 \downarrow \times 2$	$\uparrow \times 10 \downarrow \times 6$	6	8008	48048	0.3814
2μB	-6μB	$\uparrow \times 1 \downarrow \times 3$	$\uparrow \times 11 \downarrow \times 5$	4	4368	17472	0.1387
4μB	-8μB	$\uparrow \times 0 \downarrow \times 4$	$\uparrow \times 12 \downarrow \times 4$	1	1820	1820	0.0144

Table 1: Possible microstates

given by $\sum \Omega(E(A))\Omega(E(B)) = 125970$.

(a)

Reading off from Table 1, the total number of microstates at energies $E_A = -2\mu B$ and $E_B = -2\mu B$ is given by $\boxed{\Omega(E_A)\Omega(E_B) = 45760}$.

(b)

The probability that system A has energy E_A is given by:

$$P_A(E_A) = \frac{\Omega_A(E_A)\Omega_B(E_B)}{\Omega_{\text{total}}} = \frac{45760}{125970} \approx \boxed{0.3633} \tag{1}$$

(c)

$$\begin{aligned} \langle E_A \rangle &= \sum_A E_A P_A \qquad (2) \\ &= 0.1022 \times (-4\mu B) + 0.3633 \times (-2\mu B) + 0.3814 \times (0\mu B) + 0.1387 \times (2\mu B) + 0.0144 \times (4\mu B) \\ &= \boxed{-0.8004\mu B} \end{aligned}$$

(d)

Again, reading off the table, the most probable macrostate for the composite system is those with $\boxed{E_A = 0 \text{ , and } E_B = -4\mu B}$.

Problem 2: Classical Paramagnet (Gould 5.32)

(a)

The probability density and the partition function follow the Boltzmann distribution. Plugging in $E_s = -\mu B \cos\theta$ and $d\Omega = \sin\theta d\theta d\phi$ gives:

$$p(\theta,\phi)d\theta d\phi = \frac{1}{Z_1}e^{-\frac{E_s}{k_BT}} = \frac{1}{Z_1}e^{\beta\mu B\cos\theta}\sin\theta d\theta d\phi \text{ , where} \tag{3}$$

$$Z_1 = \sum_n e^{-\beta E_n} = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} e^{\beta\mu B\cos\theta}\sin\theta d\theta d\phi \tag{4}$$

(b)

Holding μ and B constants, we have $\overline{E} = -\mu B\overline{\cos\theta}$. Let's find $\overline{E}$.

$$\overline{E} = -\frac{1}{Z_1}\frac{\partial Z_1}{\partial\beta} = -\mu B\overline{\cos\theta} \Rightarrow \boxed{\overline{\cos\theta} = \frac{1}{\mu B Z_1}\frac{\partial Z_1}{\partial\beta}} \tag{5}$$

(c)

The mean magnetization is given by:

$$M = N\mu\overline{\cos\theta} \tag{6}$$

Let's compute Z_1 and $\frac{\partial Z_1}{\partial\beta}$.

$$Z_1 = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} e^{\beta\mu B\cos\theta}\sin\theta d\theta d\phi = \frac{4\pi\sinh(\beta\mu B)}{\beta\mu B} \tag{7}$$

$$\begin{aligned}\frac{\partial Z_1}{\partial\beta} &= \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \frac{\partial}{\partial\beta}e^{\beta\mu B\cos\theta}\sin\theta d\theta d\phi = \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} \mu B\cos\theta e^{\beta\mu B\cos\theta}\sin\theta d\theta d\phi \\ &= \frac{4\pi}{\beta^2\mu B}(\beta\mu B\cosh(\beta\mu B) - \sinh(\beta\mu B))\end{aligned} \tag{8}$$

Thus, $\overline{\cos\theta}$ is given by:

$$\begin{aligned}\overline{\cos\theta} &= \frac{\beta\mu B}{4\pi\sinh(\beta\mu B)} \times \frac{4\pi}{\beta^2\mu B}(\beta\mu B\cosh(\beta\mu B) - \sinh(\beta\mu B)) \\ &= \frac{1}{\beta\mu B}(\beta\mu B\coth(\beta\mu B) - 1) = \coth(\beta\mu B) - \frac{1}{\beta\mu B} = L(\beta\mu B)\end{aligned} \tag{9}$$

where $L(x)$ is the Langevin function. Therefore, the mean magnetization is obtained by plugging in Eq. 10 into Eq. 6:

$$\boxed{M = N\mu L(\beta\mu B)} \tag{10}$$

(d)

In the limit of high T, the quantity $\beta\mu B = \frac{\mu B}{k_BT} \ll 1$. Thus, for limit of high T, M can be expressed as:

$$M \approx N\mu\left(\frac{\beta\mu B}{3}\right) \Rightarrow \boxed{M = \frac{N\beta\mu^2 B}{3} \text{ , for large } T} \tag{11}$$

The susceptibility is given by:

$$\boxed{\chi = \frac{M}{B} = \frac{N\beta\mu^2}{3} \text{ , for large } T} \tag{12}$$

(e)

In the limit of low T, M is given by:

$$\boxed{M \approx N\mu\left(1 - \frac{1}{\beta\mu B}\right) = N\mu - \frac{N}{\mu B}} \tag{13}$$

(f)

The partition function of N noninteracting classical magnetic dipoles is given by:

$$Z_N = \left(\frac{4\pi\sinh(\beta\mu B)}{\beta\mu B}\right)^N \tag{14}$$

The mean energy is then given in terms of the partition function:

$$\overline{E} = -\frac{\partial Z_N}{\partial\beta} = \boxed{-\frac{N}{\beta}(\beta\mu B\coth(\beta\mu B)-1)} \tag{15}$$

The entropy is given by:

$$\begin{aligned} S &= \frac{\overline{E}}{T} + k_B\log Z_N \\ &= \boxed{Nk_B\left[\beta\mu B\coth(\beta\mu B)-1\right] + k_B\log\left[\left(\frac{4\pi\sinh(\beta\mu B)}{\beta\mu B}\right)^N\right]} \end{aligned} \tag{16}$$

At low temperature limit, i.e., as $\beta\to\infty$, the entropy diverges. The classical model of paramagnet does not agree with the third law of thermodynamics.

Problem 3: Arbitrary Spin (Gould 5.33)

Rearranging the series of Z_1 gives:

$$Z_1 = e^{-\alpha J}(1+e^{\alpha}+e^{2\alpha}+\cdots+e^{2J\alpha}) \Rightarrow e^{\alpha J}Z_1 = 1+e^{\alpha}+e^{2\alpha}+\cdots+e^{2J\alpha} \tag{17}$$

Writing the RHS of Eq. 17 in term of summation gives:

$$e^{\alpha J}Z_1 = \sum_{p=0}^{2J}(e^{\alpha})^p = \frac{(e^{\alpha})^{2J+1}-1}{e^{\alpha}-1} \tag{18}$$

Moving the exponential term in the LHS of Eq. 18 immediately gives:

$$\boxed{Z_1 = e^{-\alpha J}\frac{e^{(2J+1)\alpha}-1}{e^{\alpha}-1} = e^{-\alpha J}\frac{1-e^{(2J+1)\alpha}}{1-e^{\alpha}}} \tag{19}$$

The magnetization is given by:

$$M = Ng\mu_0\overline{m}\text{ , where }\overline{m} = \text{ mean magentic moment} \tag{20}$$

Meanwhile, we can further reduce Z_1 into:

$$Z_1 = e^{-\alpha J}\frac{1-e^{(2J+1)\alpha}}{1-e^{\alpha}} = \cosh(J\alpha)+\coth\frac{\alpha}{2}\sinh J\alpha \tag{21}$$

Now, let's calculate the mean magnetic moment.

$$\begin{aligned} \overline{m} &= \frac{1}{Z}\frac{\partial Z}{\partial\alpha} = \frac{\partial}{\partial\alpha}[\log Z] = \frac{\partial}{\partial\alpha}\log\left[\cosh(J\alpha)+\coth\frac{\alpha}{2}\sinh J\alpha\right] \\ &= \left(J+\frac{1}{2}\right)\coth\left[\left(J+\frac{1}{2}\right)\alpha\right] - \frac{1}{2}\coth\frac{\alpha}{2} = JB_J(\alpha) \end{aligned} \tag{22}$$

where $B_J(\alpha)$ is the Brillouin function. Therefore, the mean magnetization is given by:

$$\boxed{M = Ng\mu_0 JB_J(\alpha)} \tag{23}$$

Notice that $\alpha\propto T^{-1}$. At low T, $\alpha\to\infty$. Thus, $B_J\to 1$. At low temperature, $\boxed{M\to Ng\mu_0 J}$. At high temperature, $\alpha\to 0$. Thus, $B_J\to 0$ at high temperature. Therefore, $\boxed{M\to 0\text{ at high temperature}}$. As J increases, the magnetization remains constant without dropping to zero at lower temperature.

Problem 4: Negative Temperature (Sethna 6.3)

(a)

The number of accessible states of N atoms with net energy E corresponding to m excited states atoms is given by:

$$\Omega_E =_N C_m = \frac{N!}{m!(N-m)!} \tag{24}$$

The entropy is thus given by:

$$\begin{aligned} S_{\text{micro}}(E) &= k_B \log \Omega = k_B \left[\log N! - \log m! - \log(N-m)!\right] \\ &\approx k_B \left[N \log N - N - (m \log m - m) - ((N-m)\log(N-m) - (N-m))\right] \\ &= \boxed{k_B[N \log N - m \log m - (N-m)\log(N-m)]} \end{aligned} \tag{25}$$

where we have used Stirling's formula $\log n! \approx n \log n - n$.

(b)

We have the expression for inverse temperature:

$$\begin{aligned} \frac{1}{T} &= \frac{\partial S}{\partial E} = \frac{\partial S}{\partial m}\frac{\partial m}{\partial E} = k_B[-\log m + \log(N-m)] \times \frac{1}{\varepsilon} \\ &= \frac{k_B}{\varepsilon}\left[-\log\left(\frac{E}{\varepsilon} + \frac{N}{2}\right) + \log\left(\frac{N}{2} - \frac{E}{\varepsilon}\right)\right] \\ &= \frac{k_B}{\varepsilon}\left[\log\left(\frac{\frac{N}{2} - \frac{E}{\varepsilon}}{\frac{N}{2} + \frac{E}{\varepsilon}}\right)\right] \end{aligned} \tag{26}$$

Therefore, the temperature is given by:

$$\boxed{T = \frac{\varepsilon}{k_B}\left[\log\left(\frac{\frac{N}{2} - \frac{E}{\varepsilon}}{\frac{N}{2} + \frac{E}{\varepsilon}}\right)\right]^{-1}} \tag{27}$$

We can see that if $E > 0$, then the value of log will be negative, and $\boxed{T < 0}$.

(c)

i)

Let's first define the Hamiltonian to be:

$$\mathcal{H} = \begin{pmatrix} -\varepsilon/2 & 0 \\ 0 & \varepsilon/2 \end{pmatrix} \tag{28}$$

In canonical ensemble,

$$Z_{\text{canon}} = \text{Tr}(e^{-\beta\mathcal{H}}) = \sum_{E_n = \pm\varepsilon/2} e^{-\beta E_n} = e^{\frac{1}{2}\beta\varepsilon} + e^{-\frac{1}{2}\beta\varepsilon} = 2\cosh\left(\frac{\beta\varepsilon}{2}\right) \tag{29}$$

Let the probability density be $\rho = \frac{1}{Z}e^{-\beta\mathcal{H}} = \left[2\cosh\left(\frac{\beta\varepsilon}{2}\right)\right]^{-1}\begin{pmatrix} e^{\beta\varepsilon/2} & 0 \\ 0 & e^{-\beta\varepsilon/2}\end{pmatrix}$. Then the energy is given by:

$$\begin{aligned} E_{\text{canon}} &= \text{Tr}(\mathcal{H}\rho) = \frac{1}{Z_{\text{canon}}}\text{Tr}\left[\begin{pmatrix} -\varepsilon/2 & 0 \\ 0 & \varepsilon/2 \end{pmatrix}\begin{pmatrix} e^{\frac{\beta\varepsilon}{2}} & 0 \\ 0 & e^{-\frac{\beta\varepsilon}{2}}\end{pmatrix}\right] \\ &= \frac{1}{2\cosh(\beta\varepsilon/2)}\left[-\frac{\varepsilon}{2}\left(e^{\beta\varepsilon/2} - e^{-\beta\varepsilon/2}\right)\right] = -\frac{\varepsilon}{2}\frac{2\sinh(\beta\varepsilon/2)}{2\cosh(\beta\varepsilon/2)} = -\frac{\varepsilon}{2}\tanh\left(\frac{\beta\varepsilon}{2}\right) \end{aligned} \tag{30}$$

The entropy is given by:

$$S_{\text{canon}} = \text{Tr}\Big(\rho(-k_B \log\rho)\Big) = -k_B \text{Tr}\Big(\rho\log\rho\Big) = -\frac{k_B}{Z}\left[e^{\beta\varepsilon/2}\log\left(\frac{e^{\beta\varepsilon/2}}{Z}\right) + e^{-\beta\varepsilon/2}\log\left(\frac{e^{-\beta\varepsilon/2}}{Z}\right)\right] \tag{31}$$

In summary, writing Z, E, S in terms of traces, we have:

$$\begin{aligned} Z_{\text{canon}} &= \text{Tr}(e^{-\beta\mathcal{H}}) && (32)\\ E_{\text{canon}} &= \text{Tr}(\rho\mathcal{H}) && (33)\\ S_{\text{canon}} &= -k_B \text{Tr}\Big(\rho \log \rho\Big) && (34) \end{aligned}$$

ii)

In terms of thermodynamics, we have:

$$\begin{aligned} A &= -k_B T \log Z && (35)\\ S_{\text{canon}} &= \frac{\partial A}{\partial T} = -k_B\left[\frac{\partial}{\partial T}(T\log Z)\right] = -k_B\left[-\log Z - \frac{1}{k_B T}\frac{\varepsilon}{2}\tanh\left(\frac{\beta\varepsilon}{2}\right)\right] = k_B \log Z + \frac{E}{T} && (36)\\ E_{\text{canon}} &= A + TS = -\frac{\varepsilon}{2}\tanh\left(\frac{\beta\varepsilon}{2}\right) && (37) \end{aligned}$$

Comparing these expressions with the above results, we can directly see that the thermodynamical fomulae agree with the statistical traces.

(d)

From the expression $E = -\frac{\varepsilon}{2}\tanh\left(\frac{\varepsilon}{2k_B T}\right)$, we see that $E \propto \tanh\left(\frac{1}{T}\right)$. As $T \to \infty$, $\boxed{E \propto \tanh\left(\frac{1}{T}\right) \to 0}$. Thus, in canonical ensemble, we can't access the negative temperature.

(e)

The entropy of N particles is straightforward:

$$\boxed{S_N = N\frac{E}{T} + Nk_B \log Z} \tag{38}$$

Let's rewrite S as $S_N = \frac{NE}{T} + Nk_B \log\left[\sum e^{-E_n/k_B T}\right]$. Then we can clearly see that

$$S_N(T) \to \begin{cases} Nk_B \log 2 & , \text{ when } T \to \infty \\ 0 & , \text{ when } T \to 0 \end{cases} \tag{39}$$

Thus, $S(T=\infty) - S(T=0) = Nk_B \log 2$. This corresponds to the conceptual explanation that as temperature goes to infinity, all microstates become equally likely.

Before calculating the canonical entropy, following expressions will help:

$$\begin{aligned} E &= -N\frac{\varepsilon}{2}\tanh\left(\frac{\beta\varepsilon}{2}\right) \Rightarrow \frac{\beta\varepsilon}{2} = \tanh^{-1}\left(-\frac{2E}{N\varepsilon}\right) = -\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right) && (40)\\ Z &= 2\cosh\left(\frac{\beta\varepsilon}{2}\right) = 2\cosh\left[-\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right)\right] = 2\cosh\left[\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right)\right] && (41)\\ T &= \frac{\varepsilon}{k_B}\left[\log\left(\frac{\frac{N}{2}-\frac{E}{\varepsilon}}{\frac{N}{2}+\frac{E}{\varepsilon}}\right)\right]^{-1} = \frac{\varepsilon}{k_B}\left[\log\left(\frac{1-\frac{2E}{N\varepsilon}}{1+\frac{2E}{N\varepsilon}}\right)\right]^{-1} \Rightarrow \frac{1}{T} = \frac{k_B}{\varepsilon}\log\left(\frac{1-\frac{2E}{N\varepsilon}}{1+\frac{2E}{N\varepsilon}}\right) && (42)\\ \tanh^{-1} x &= \frac{1}{2}\log\left(\frac{1+x}{1-x}\right) && (43) \end{aligned}$$

The canonical entropy is given by:

$$S_{\text{canon}} = Nk_B \log Z + N\frac{E}{T} \tag{44}$$

We plug in the expressions above to Eq. 44, let $x \equiv \frac{2E}{N\varepsilon}$, and use the fact that

$$\begin{aligned} 1+x &= 1 + \frac{2E}{N\varepsilon} = \frac{2m}{N} && (45)\\ 1-x &= \frac{2(N-m)}{N} && (46) \end{aligned}$$

. Then we get:

$$\begin{aligned}
S_{\text{canon}}(T(E)) &= Nk_B \log\left[2\cosh\left(\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right)\right)\right] - \frac{N}{T}\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right) \qquad (47)\\
&= Nk_B \log\left[2\cosh\left(\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right)\right)\right] - \frac{2k_B E}{\varepsilon}\tanh^{-1}\left(\frac{2E}{N\varepsilon}\right)\\
&= Nk_B \log\left[2\cosh\left(\tanh^{-1}(x)\right)\right] - \frac{2k_B E}{\varepsilon}\tanh^{-1}(x)\\
&= Nk_B \log\left[2\cosh\left[\frac{1}{2}\log\left(\frac{1+x}{1-x}\right)\right]\right] - \frac{2k_B E}{\varepsilon}\tanh^{-1}\left[\frac{1}{2}\log\left(\frac{1+x}{1-x}\right)\right]\\
&= Nk_B\left[\log 2 - \frac{1}{2}(1+x)\log(1+x) - \frac{1}{2}(1-x)\log(1-x)\right]\\
&= k_B\left[N\log N - m\log m - (N-m)\log(N-m)\right] = S_{\text{micro}}(E) \qquad (48)
\end{aligned}$$

phew! Therefore,

$$\boxed{S_{\text{canon}}(T(E)) = S_{\text{micro}}(E)\text{ , for large } N.} \qquad (49)$$

In small N, we observe that the microcanonical entropy is smaller than canonical entropy, because for microcanonical ensemble, we have the total energy specified, whereas for canonical ensemble, we have more uncertainty in the total energy because the ensemble is connected to a heat bath. Since we have more unknowns for canonical ensemble, the canonical entropy is greater than microcanonical entropy for $N = 50$.

(f)

The mean of energy squared is given by:

$$\langle E^2\rangle = -\frac{\partial^2 \log Z}{\partial\beta^2} = \frac{1}{2}\varepsilon\frac{\partial}{\partial\beta}\tanh\left(\frac{\beta\varepsilon}{2}\right) = \frac{1}{4}\varepsilon^2\operatorname{sech}^2\left(\frac{\beta\varepsilon}{2}\right) \qquad (50)$$

Thus, RMS energy is given by:

$$E_{RMS} = \sqrt{\langle E^2\rangle} = \boxed{\frac{\varepsilon N^{1/2}}{2}\operatorname{sech}\left(\frac{\beta\varepsilon}{2}\right)} \qquad (51)$$

At temperature obtained at part (b), we have:

$$\begin{aligned}
T(E) &= \frac{\varepsilon}{k_B}\left[\log\left(\frac{1-x}{1+x}\right)\right]^{-1} = \frac{\varepsilon}{k_B}\left[\log\left(\frac{N-m}{m}\right)\right]^{-1} \qquad (52)\\
\frac{\beta\varepsilon}{2} &= \frac{\varepsilon}{2k_B T} = \frac{1}{2}\log\left(\frac{N-m}{m}\right) \qquad (53)
\end{aligned}$$

Evaluating E_{RMS} at the above temperature gives:

$$E_{RMS}(T(E)) = \frac{\varepsilon N^{1/2}}{2}\operatorname{sech}\left(\frac{1}{2}\log\left(\frac{N-m}{m}\right)\right) = \boxed{\frac{\varepsilon}{\sqrt{N}}\sqrt{m(N-m)}} \qquad (54)$$

Remember that

$$m = \frac{E}{\varepsilon} + \frac{N}{2} \Rightarrow E = \varepsilon\left(m - \frac{N}{2}\right). \qquad (55)$$

We evaluate E_{RMS}/E to compare the fluctuation and E.

$$\frac{E_{RMS}}{E} = \frac{\varepsilon}{\sqrt{N}}\frac{\sqrt{m(N-m)}}{\varepsilon(m-N/2)} \qquad (56)$$

At large N, Eq. 56 reduces to:

$$\frac{E_{RMS}}{E} \approx \frac{\varepsilon}{\sqrt{N}}\frac{\sqrt{N}\sqrt{m}}{\varepsilon(N/2)} = \frac{2\sqrt{m}}{N} \qquad (57)$$

Therefore, we see that as $\boxed{N \to \infty, \frac{E_{RMS}}{E} \to 0}$.

Problem 5: Zipf's Law (Sethna 6.24)

(a)

A message is thought to have more information if it occurs more rarely, whereas it has less information if it occurs commonly. For example, the word **something** has less information than **primeval**. Thus, we look for a function $I(i)$ such that it gives 0 if the probability $p_i = 1$, and blows up as the probability $p_i \to 0$. The function that satisfies the condition is given by:

$$\boxed{I(i) = k_S \log \frac{1}{p_i}} \tag{58}$$

where k_S is some coefficient.

In a random series of N words, we simply sum the information of each word, weighted by its rank. That is,

$$\boxed{I = k_S \sum_j N_j \log \frac{1}{p_j}} \tag{59}$$

(b)

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial N_j} &= \frac{\partial}{\partial N_j}\left[k_S N_j \log\left(\frac{N}{N_j}\right) - \beta(N_j c_j - E) - \lambda(N_j - N)\right] \\ &= k_S \log\left(\frac{N}{N_j}\right) - k_S - \beta c_j - \lambda \\ &= k_S \log\left(\frac{N}{N_j}\right) - k_S - \beta(k_S \log j + c_0) - \lambda = 0 \end{aligned} \tag{60}$$

Setting the above equation to zero and solving for N_j gives:

$$k_S + \beta(k_S \log j + c_0) + \lambda = k_S \log\left(\frac{N}{N_j}\right) \tag{61}$$

$$e^{k_S + \beta c_0 + \lambda}\left(e^{\log j}\right)^{\beta k_S} = \left(e^{\log N/N_j}\right)^{k_S} \tag{62}$$

$$\exp\left[1 + \frac{\beta c_0 + \lambda}{k_S}\right] j^\beta = \frac{N}{N_j} \tag{63}$$

$$\boxed{N_j = \frac{N}{j^\beta} \exp\left[-1 - \frac{\beta c_0 + \lambda}{k_S}\right]} \tag{64}$$

(c)

$$N = \sum_j N_j = \sum_j \frac{N}{j^\beta} \exp\left[-1 - \frac{\beta c_0 + \lambda}{k_S}\right] = \zeta(\beta) N \exp\left[-1 - \frac{\beta c_0 + \lambda}{k_S}\right] \tag{65}$$

Solving for λ, we get

$$1 = \zeta(\beta) \exp\left[-1 - \frac{\beta c_0 + \lambda}{k_S}\right] \tag{66}$$

$$\log\left(\frac{1}{\zeta(\beta)}\right) = -1 - \frac{\beta c_0 + \lambda}{k_S} \tag{67}$$

$$\boxed{\lambda = k_S \log\left(\frac{1}{\zeta(\beta)}\right) + k_S + \beta c_0} \tag{68}$$

Plugging in λ to Eq. 64 gives:

$$N_j = \frac{N}{j^\beta} \exp\left[-1 - \frac{\beta c_0}{k_S} + \left(\log\left(\frac{1}{\zeta(\beta)} + 1 + \frac{\beta c_0}{k_S}\right)\right)\right] = \boxed{\frac{N}{j^\beta \zeta(\beta)}} \tag{69}$$

(d)

We are to calculate the effort E. The ingredients we have are:

$$
\begin{aligned}
E &= \sum_j N_j C_j && (70)\\
C_j &= k_S \log j + c_0 && (71)\\
N_j &= \frac{N}{j^\beta \zeta(\beta)} && (72)\\
\zeta(\beta) &= \sum_{j=1}^{\infty} j^{-\beta} && (73)\\
\frac{\partial j^{-\beta}}{\partial \beta} &= -j^{-\beta}\log j && (74)
\end{aligned}
$$

Now, the effort E is given by:

$$
\begin{aligned}
E &= \sum_j N_j C_j = \sum_{j=1}^{\infty} [k_S \log j + c_0]\left[\frac{N}{j^\beta \zeta(\beta)}\right] = \sum_{j=1}^{\infty} \frac{k_S N \log j}{j^\beta \zeta(\beta)} + \sum_{j=1}^{\infty} \frac{c_0 N}{j^\beta \zeta(\beta)} \qquad (75)\\
&= \frac{k_S N}{\zeta(\beta)} \sum_{j=1}^{\infty} \frac{\log j}{j^\beta} + \frac{c_0 N}{\zeta(\beta)} \sum_{j=1}^{\infty} j^{-\beta} = -\frac{k_S N}{\zeta(\beta)} \sum_{j=1}^{\infty} \frac{\partial j^{-\beta}}{\partial \beta} + \frac{c_0 N}{\zeta(\beta)} \zeta(\beta)\\
&= -\frac{k_S N}{\zeta(\beta)} \frac{\partial \zeta(\beta)}{\partial \beta} + c_0 N = \boxed{\frac{k_S N}{\zeta(\beta)} \sum_{n=2}^{\infty} \frac{\log n}{n^\beta} + c_0 N}
\end{aligned}
$$

(e)

The information I is given by:

$$
\begin{aligned}
I &= -k_S \sum_j N_j \log\left(\frac{N_j}{N}\right) = -k_S \sum_j \frac{N}{j^\beta \zeta(\beta)} \log\left(\frac{1}{j^\beta \zeta(\beta)}\right) \qquad (76)\\
&= k_S \sum_j \frac{N}{j^\beta \zeta(\beta)} \log j^\beta + k_S \sum_j \frac{N}{j^\beta \zeta(\beta)} \log \zeta(\beta)\\
&= \frac{N k_S \beta}{\zeta(\beta)} \sum_j j^{-\beta} \log j + \frac{N k_S}{\zeta(\beta)} \log \zeta(\beta) \sum_j j^{-\beta} = -\frac{N k_S \beta}{\zeta(\beta)} \sum_j \frac{\partial j^{-\beta}}{\partial \beta} + \frac{N k_S}{\zeta(\beta)} \log[\zeta(\beta)]\zeta(\beta)\\
&= -\frac{N k_S \beta}{\zeta(\beta)} \frac{\partial \zeta(\beta)}{\partial \beta} + k_S N \log \zeta(\beta) = \boxed{\frac{N k_S \beta}{\zeta(\beta)} \sum_{n=2}^{\infty} \frac{\log n}{n^\beta} + k_S N \log \zeta(\beta)}
\end{aligned}
$$

(f)

Attached below as a Mathematica notebook.

(g)

Attached below as a Mathematica notebook.

Problem 6: Freely Jointed-Chain (FJC) Model of a Polymer

(a)

First notice that the total length L of a polymer is determined by summing up all the $\hat{\mathbf{z}}$ components of the length $d\hat{\mathbf{t}}_i$ of individual monomers:

$$
L = \sum_i d\hat{\mathbf{t}}_i \cdot \hat{\mathbf{z}} = d \sum_i \hat{\mathbf{t}}_i \cdot \hat{\mathbf{z}} \qquad (77)
$$

The partition function of an individual configuration is given by:

$$e^{\beta FL} = \exp\left[\frac{1}{k_B T} Fd \sum_i \hat{\mathbf{z}} \cdot \hat{\mathbf{t}}_i\right] \tag{78}$$

Thus, the probability that the polymer is in a state such that each monomer points to a certain direction $\hat{t}_i$ is given by:

$$\boxed{P(\{\hat{\mathbf{t}}_i\}) = \frac{1}{Z(T,F)} \exp\left[\frac{Fd}{k_B T} \sum_i \hat{\mathbf{z}} \cdot \hat{\mathbf{t}}_i\right]} \tag{79}$$

where Z is the partition function.

(b)

The tricky part here is that the length $L(s)$ of the polymer can be of any value between $0 \leq L(s) \leq Nd$, depending on the angles of monomers with respect to $\hat{\mathbf{z}}$. The partition function is written as:

$$Z(T,F) = \sum_s \exp\left[\frac{FL(s)}{k_B T}\right] \tag{80}$$

where s runs over all possible microstates. $L(s)$ is expressed as:

$$L(s) = d\sum_i \hat{\mathbf{t}}_i \cdot \hat{\mathbf{z}} = d\sum_i \cos\theta_i \tag{81}$$

where θ_i is the angle between $\hat{\mathbf{t}}_i$ and $\hat{\mathbf{z}}$. Plugging in the expression into Eq. 80 gives

$$\begin{aligned} Z(T,F) &= \int_{\theta_i=0}^{\pi}\int_{\phi_i=0}^{2\pi} \exp\left[\frac{Fd}{k_B T}\sum_i \cos\theta_i\right] \sin\theta_i d\theta_i d\phi_i \\ &= \prod_{i=1}^{N} \int_{\theta_i=0}^{\pi}\int_{\phi_i=0}^{2\pi} \exp\left[\frac{Fd}{k_B T}\cos\theta_i\right]\sin\theta_i d\theta_i d\phi_i \\ &= 2\pi\left(\int_{\theta=0}^{\pi}\exp\left[\frac{Fd}{k_B T}\cos\theta\right]\sin\theta d\theta\right)^N = \boxed{\left[\frac{4\pi k_B T}{Fd}\sinh\left(\frac{Fd}{k_B T}\right)\right]^N} \end{aligned} \tag{82}$$

The free energy A is given by:

$$\boxed{A = -k_B T\log(Z)\ ,\ \text{where } Z = \left[\frac{4\pi k_B T}{Fd}\sinh\left(\frac{Fd}{k_B T}\right)\right]^N} \tag{83}$$

(c)

$$\boxed{\langle L\rangle = \beta\frac{\partial}{\partial F}\log Z = \frac{N}{Fk_B T}\left[\frac{dF}{k_B T}\coth\left(\frac{dF}{k_B T}\right) - 1\right]} \tag{84}$$

(d)

Let's clean up the expression at part c using $\beta = \frac{1}{k_B T}$. For small force, we can expand $\coth x \approx \frac{1}{x} + \frac{x}{3}$

$$\begin{aligned} \langle L\rangle &= \frac{N}{\beta F}\left[\beta dF\coth(\beta dF) - 1\right] = Nd\coth(\beta dF) - \frac{N}{\beta F} & (85)\\ \Rightarrow \frac{1}{Nd}\langle L\rangle &= \coth(\beta dF) - \frac{1}{\beta dF} \approx \frac{1}{\beta dF} + \frac{\beta dF}{3} - \frac{1}{\beta dF} = \frac{\beta dF}{3} & (86)\\ \Rightarrow \langle L\rangle &= \boxed{\frac{N\beta d^2 F}{3}\ ,\ \text{when } F \text{ is small}} & (87) \end{aligned}$$

Setting $k \equiv -\frac{3}{N\beta d^2}$, $x \equiv \langle L \rangle$ and rearranging in terms of force, we get the expression

$$\boxed{F = \frac{3\langle L \rangle}{N\beta d^2} = -kx} \tag{88}$$

which is a form of Hooke's Law.

At large force limit, $\coth(\beta dF) \to 1$. Thus the expression reduces to:

$$\boxed{\langle L \rangle \approx Nd - \frac{N}{F\beta} \text{ , when } F \text{ is large.}} \tag{89}$$

(e)

The mean energy is given by:

$$\langle E \rangle = -\frac{\partial \log Z}{\partial \beta} = -\frac{\partial}{\partial \beta} \log \left[\frac{4\pi}{\beta dF} \sinh(\beta dF)\right]^N = \boxed{\frac{N}{\beta} - NdF \coth(\beta dF)} \tag{90}$$

The entropy is given by:

$$S = k_B \frac{\partial}{\partial T} T \log Z = \boxed{-\frac{dFN}{T} \coth(\beta dF) + k_B N + k_B \log \left[\left(\frac{4\pi \sinh(\beta dF)}{\beta dF}\right)^N\right]} \tag{91}$$

Let's define the information and effort first.

In[38]:=

```
Info = (n ks β / Zeta[β]) Sum[Log[n] / n^β, {n, 2, ∞}] + ks n Log[Zeta[β]];
Effort = (n ks / Zeta[β]) Sum[Log[n] / n^β, {n, 2, ∞}] + c0 n;
```

Part (f)

We are to plot $\frac{I(\beta)}{E(\beta)}$ with $c_0 = 0$.

For now, the values of N and k_S are irrelevant, but it will become useful later, so let's define them as well.

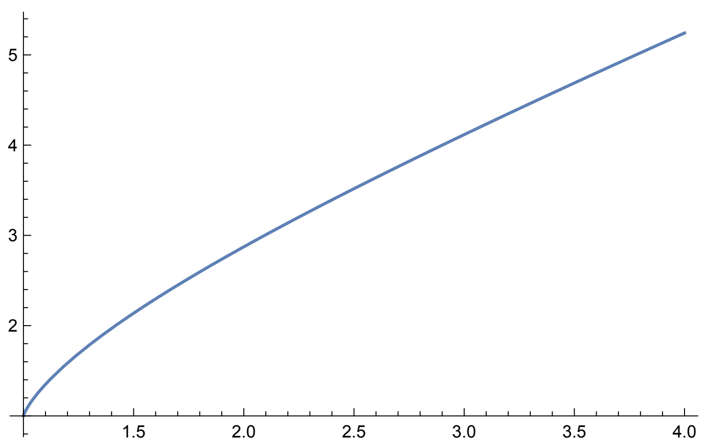
In[42]:=

```
n = 10;
ks = 1;
```

In[44]:=

```
Plot[Info / (Effort /. {c0 → 0}), {β, 1, 4}]
```

Out[44]=



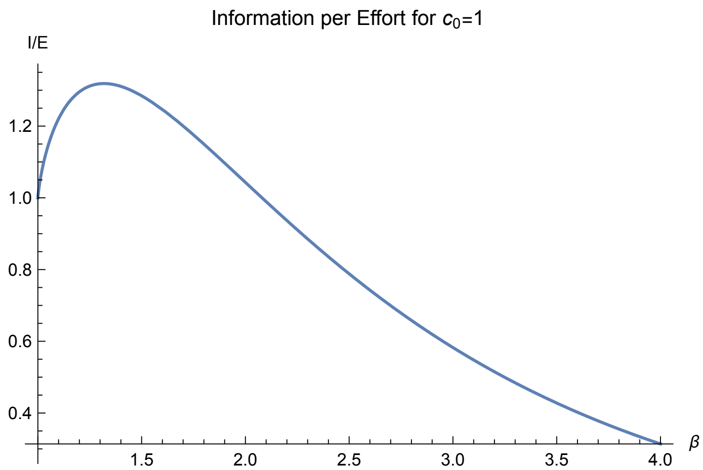
We notice here that when $c_0 = 0$, the maximum is at $\beta = 4$, and it keeps increasing. This represents an unphysical state, as we are here setting the extra effort to recognize a new word to be 0.

Part (g)

Now we are plotting with $c_0 = 1$ and $c_0 = 2$.

In[54]:=
```
Plot[Info / (Effort /. {c0 → 1}), {β, 1, 4},
 PlotLabel → "Information per Effort for c₀=1", AxesLabel → {β, "I/E"}]
```

Out[54]=

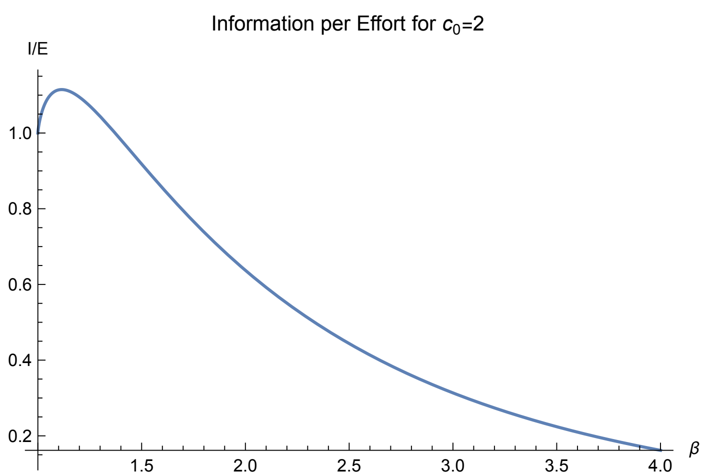


In[53]:=
```
FindMaximum[Info / (Effort /. {c0 → 1}), {β, 1.1}]
```

Out[53]= {1.31863, {β → 1.31863}}

In[56]:=
```
Plot[Info / (Effort /. {c0 → 2}), {β, 1, 4},
 PlotLabel → "Information per Effort for c₀=2", AxesLabel → {β, "I/E"}]
```

Out[56]=



In[57]:=
```
FindMaximum[Info / (Effort /. {c0 → 2}), {β, 1.1}]
```

Out[57]= {1.1148, {β → 1.1148}}