8. *Statistical Mechanics and Thermodynamics* (Spring 2006)

(a) A system consists of N particles, each of which can exist in two states, with energies ϵ_0 and ϵ_1, respectively. Given that the total energy of this system is U, what is its entropy?

(b) Obtain the expression for the entropy in the limit that N is large.

(c) Now, give an expression for the temperature of this system, as a function of U and the energies of the single particle states. Does this expression have any properties that require some discussion?

Stirling's formula: $n! \approx (\frac{n}{e})^n$, when n is large.

a. The single particle partition function is

$$\zeta = \sum_r e^{-\beta\epsilon_r} = e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}$$

$$\Rightarrow Z = \frac{\zeta^N}{N!} = \frac{1}{N!}\left(e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}\right)^N$$

$$S = K(\ln(Z) + \beta U) = K\left[N\ln\left(e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}\right) - \ln(N!) + \beta U\right]$$

b. Using Stirling's Formula, $\ln(N!) \cong N\ln(\frac{N}{e}) = N\ln(N) - N$

$$\Rightarrow S \cong K\left[N\ln\left(e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}\right) - N\ln(N) + N + \beta U\right]$$

c. $U = -\dfrac{\partial\ln(Z)}{\partial\beta}$ where $\ln(Z) = N\ln\left(e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}\right) - \ln(N!)$

$$U = N\,\frac{\epsilon_0 e^{-\beta\epsilon_0} + \epsilon_1 e^{-\beta\epsilon_1}}{e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}}$$

Now group like terms to solve for β

$$U\left(e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}\right) = N\left(\epsilon_0 e^{-\beta\epsilon_0} + \epsilon_1 e^{-\beta\epsilon_1}\right)$$

$$(U - N\epsilon_0)e^{-\beta\epsilon_0} = (N\epsilon_1 - U)e^{-\beta\epsilon_1}$$

$$e^{\beta(\epsilon_1 - \epsilon_0)} = \frac{N\epsilon_1 - U}{U - N\epsilon_0}$$

$$\beta(\epsilon_1 - \epsilon_0) = \ln\left(\frac{N\epsilon_1 - U}{U - N\epsilon_0}\right)$$

$$T = \frac{\epsilon_1 - \epsilon_0}{K}\left[\ln\left(\frac{N\epsilon_1 - U}{U - N\epsilon_0}\right)\right]^{-1}$$

This expression has the property that it is negative if $N\epsilon_1 - U < U - N\epsilon_0 \Leftrightarrow U > \frac{1}{2}N(\epsilon_0 + \epsilon_1)$, which is a characteristic of systems with an upper limit to their total energy (see Reif page 105).