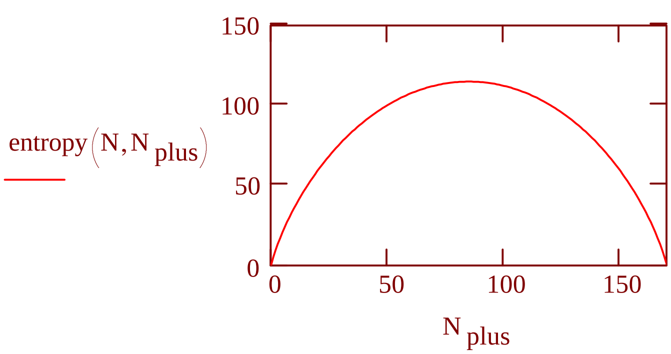
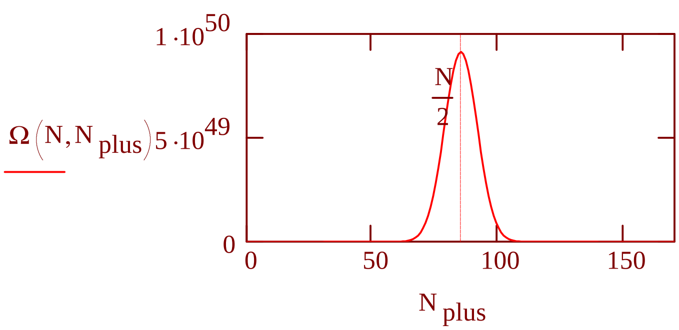
Statistical Physics Computer Lab. #2b
Two-State Model, Negative Temperatures, and the Schottky Hump

We consider the two-state model. Each atom has an energy of $-\varepsilon$ or ε. There are N atoms and the total energy is U. Since $N = N_{plus} + N_{minus}$ and $U = \varepsilon(N_{plus} - N_{minus})$ we can solve for the numbers: $N_{plus} = 1/2(N + U/\varepsilon)$ and $N_{minus} = 1/2(N - U/\varepsilon)$. In the microcanonical ensemble the number of microstates corresponding to the total energy U and the number of atoms N is $\Omega = N!/N_{plus}!N_{minus}!$. The entropy is, according to the Boltzmann postulate, $S = k_B \ln W$. In what follows we express the entropy in units of k_B and the energy in units of ε.

$$N := 170 \qquad N_{plus} := 0 .. N$$

$$\Omega(N, N_{plus}) := \frac{N!}{N_{plus}! \cdot (N - N_{plus})!} \qquad \text{entropy}(N, N_{plus}) := \ln(\Omega(N, N_{plus}))$$





Note the huge number of microstates for $N_{plus} = N_{minus} = N/2$

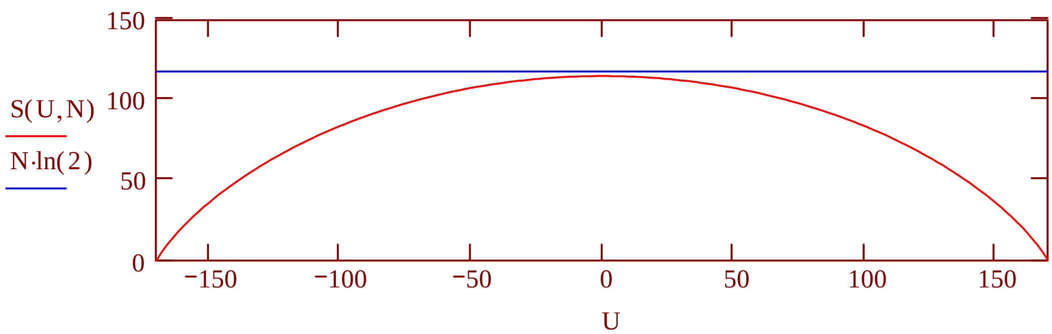
Next we define the entropy as function of energy and number of atoms. Note that U stands for U/ε.

$$N_{plus}(U,N) := \frac{1}{2}\cdot(N+U) \qquad S(U,N) := \text{entropy}\left(N, N_{plus}(U,N)\right)$$

To compute the entropy, U and N must be either both even integers or both odd integers. Furthermore: -N < U < N. Examples:

$S(5,97) = 64.59195$ $\qquad$ $S(168,170) = 5.1358$

$U := -170, -168 .. 170$ $\qquad$ $N := 170$



Note the maximum entropy is Nln(2) and it occurs for U = 0 or $N_{plus} = N_{minus}$.

The temperature is obtained from 1/T = dS/dU. We are going to obtained the derivative numerically 1/T = ΔS/ΔU with the smallest possible ΔU = 2. The temperature is negative for U > 0 when $N_{plus} > N_{minus}$. The temperature is positive for U <0 when $N_{plus} < N_{minus}$.

$$T(U,N) := \frac{1}{\dfrac{S(U+2,N) - S(U,N)}{2}}$$

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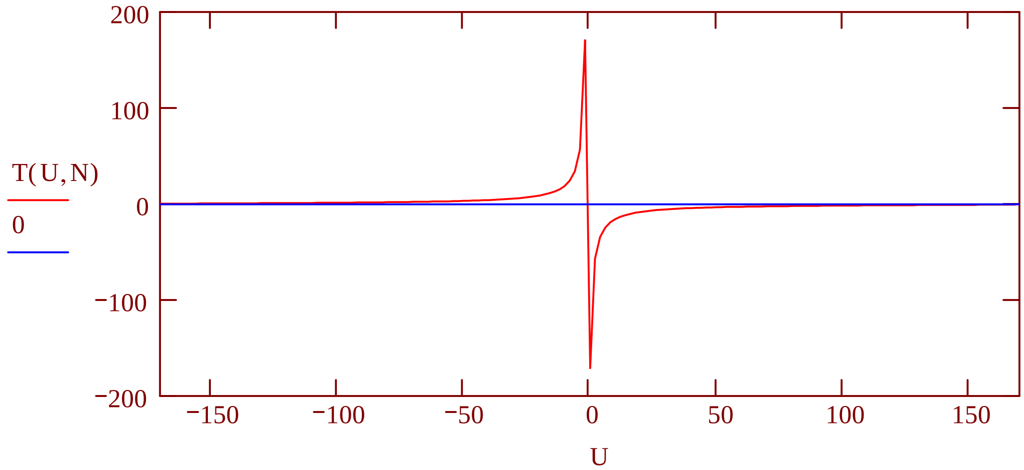

The heat capacity is C = dU/dT is obtained numerically as: ΔU/ΔT with the smallest possible ΔU =2. Note C vs T exhibits the famous Schottky hump.

$$C(U,N) := \frac{2}{T(U+2,N) - T(U,N)}$$