TWO-STATE PARAMAGNET: NUMERICAL SOLUTION

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Reference: Daniel V. Schroeder, *An Introduction to Thermal Physics*, (Addison-Wesley, 2000) - Problems 3.17 - 3.18.

We can apply the formulas for entropy, temperature and heat capacity to a real-life system by looking at a two-state paramagnet. This is a system of N magnetic dipoles which, when placed in a magnetic field B, align themselves so that their magnetic moment μ points either parallel or antiparallel to the field. The energy of a dipole that is aligned with the field is lower, and we'll call it $-\mu B$, so that the antiparallel dipole has energy $+\mu B$, and the total energy of the system is

$$U=\mu B\left(N_{\downarrow}-N_{\uparrow}\right)=\mu B\left(N-2N_{\uparrow}\right) \tag{1}$$

where an up arrow indicates parallel alignment and a down arrow antiparallel.

The net magnetization is then

$$M=\mu\left(N_{\uparrow}-N_{\downarrow}\right)=-\frac{U}{B} \tag{2}$$

The multiplicity of states is the same as a set of N coins with $N_{\uparrow}$ heads, so

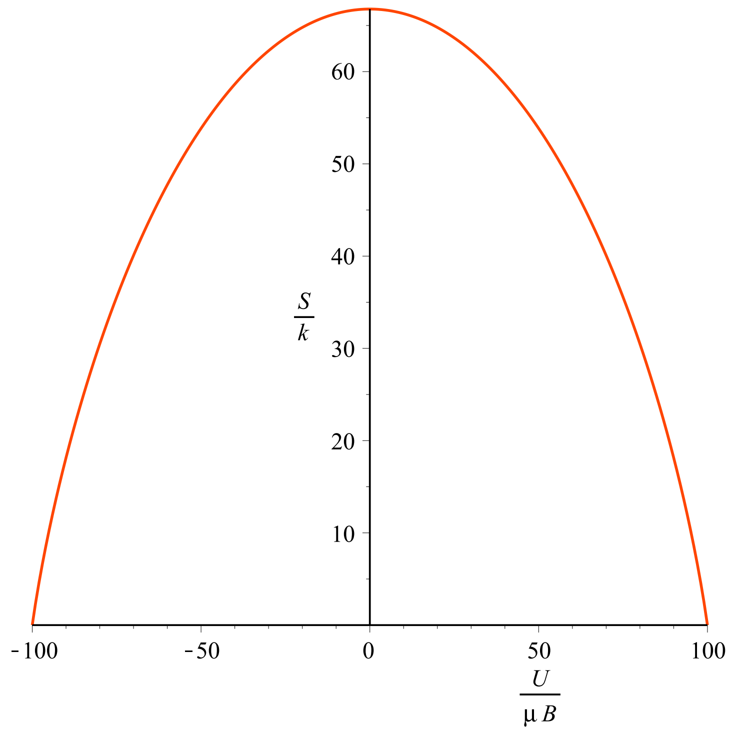
$$\Omega=\binom{N}{N_{\uparrow}}=\frac{N!}{N_{\uparrow}!\left(N-N_{\uparrow}\right)!} \tag{3}$$

For small systems, we can find the entropy directly as

$$\frac{S}{k}=\ln\Omega \tag{4}$$

For $N_{\uparrow}=98$, we get $U/\mu B=-96$, $M/N\mu=0.96$, $\Omega=4950$ and $S/k=8.507$.

For each value of $N_{\uparrow}$ from 0 up to N, we can evaluate U and S from the formulas above and then plot S versus U (I used Maple for the plot):



For $-100 \leq U/\mu B < 0$, the curve is a 'normal' entropy curve in that the entropy increases with increasing energy, and the curve is concave down.

From this we can get the temperature

$$\frac{1}{T} = \frac{\partial S}{\partial U} \tag{5}$$

Thus the temperature increases with energy in the region $-100 \leq U/\mu B < 0$. At $U = 0$, however, the derivative is zero implying an infinite temperature, and for $U > 0$, the slope is negative, indicating a negative temperature. Since, in this case, negative temperatures occur at higher energies than positive temperatures, we have to interpret a negative temperature as actually being higher than a positive one, in fact, higher than an 'infinite' positive temperature.

In this case, it's probably better to use the entropy of the system as a physical measure of what's going on, since the second law implies that the system will tend to the energy with the greatest entropy, which is $U = 0$. At this energy, there are equal numbers of up and down dipoles, so the system is maximally randomized.

For a system with $N = 100$, we can approximate 5 by taking finite differences. Thus for a given value of $N_\uparrow$ we can estimate the temperature as

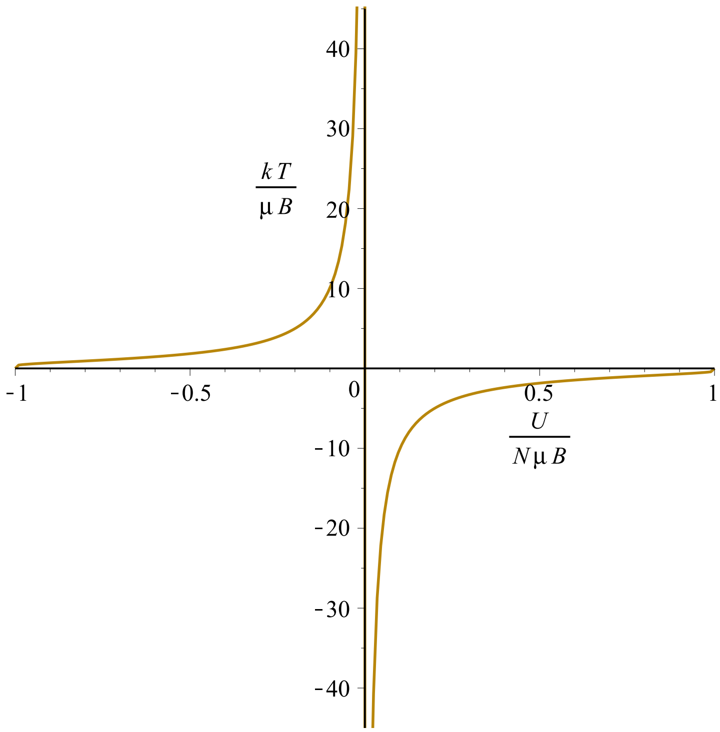
$$T\left(N_{\uparrow}\right) = \frac{\Delta U}{\Delta S} \tag{6}$$

$$= \frac{U\left(N_{\uparrow}+1\right)-U\left(N_{\uparrow}-1\right)}{S\left(N_{\uparrow}+1\right)-S\left(N_{\uparrow}-1\right)} \tag{7}$$

For $N_{\uparrow}=98$, we get

$$T(98)=\frac{U(99)-U(97)}{S(99)-S(97)}=0.541\frac{\mu B}{k} \tag{8}$$

This allows us to plot temperature versus energy:



We can see the flip over from $+\infty$ to $-\infty$ as the energy increases through zero.

The heat capacity can be obtained similarly as

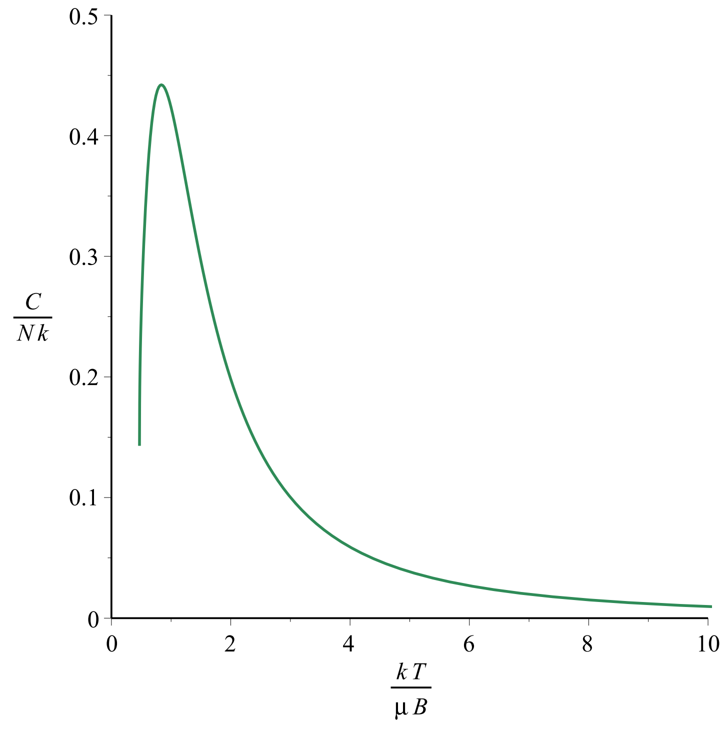
$$C = \frac{\Delta U}{\Delta T} \tag{9}$$

$$= \frac{U\left(N_{\uparrow}+1\right)-U\left(N_{\uparrow}-1\right)}{T\left(N_{\uparrow}+1\right)-T\left(N_{\uparrow}-1\right)} \tag{10}$$

where we use 7 to calculate the temperatures. For $N_{\uparrow}=98$ we have

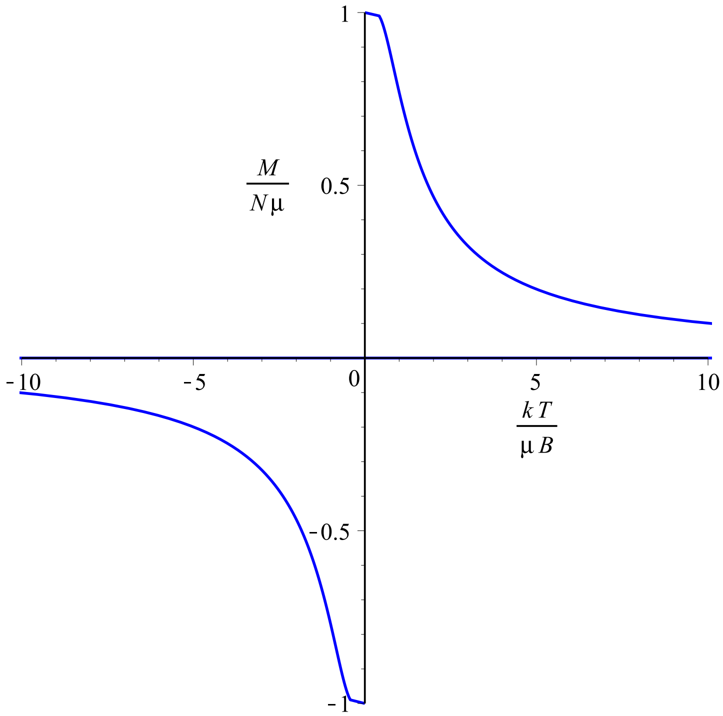
$$C(98) = 0.310Nk \tag{11}$$

The plot of C versus temperature is



[The plot does actually extend down to 0 at $T = 0$ if we use the analytic solution, but because we're dealing with discrete values of $N_\uparrow$, it cuts out early.] This curve is similar in shape to that of an Einstein solid at low temperatures.

Finally, we can plot the magnetization as a function of temperature:



If we start off with $T>0$ and lower the temperature towards zero, the magnetization gradually increases until at $T=0$, the system is frozen into the state where all dipoles are parallel to the field. As we increase T to $+\infty$, we approach maximum randomness with equal numbers of dipoles pointing up and down so $M\rightarrow0$. Increasing the temperature beyond $+\infty$ so it becomes negative (starting at $-\infty$) the magnetization again increases, but now the dipoles are aligned antiparallel to the field, eventually saturating as $T\rightarrow0$ from the negative side.

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