

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

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

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

The net magnetization is then

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

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

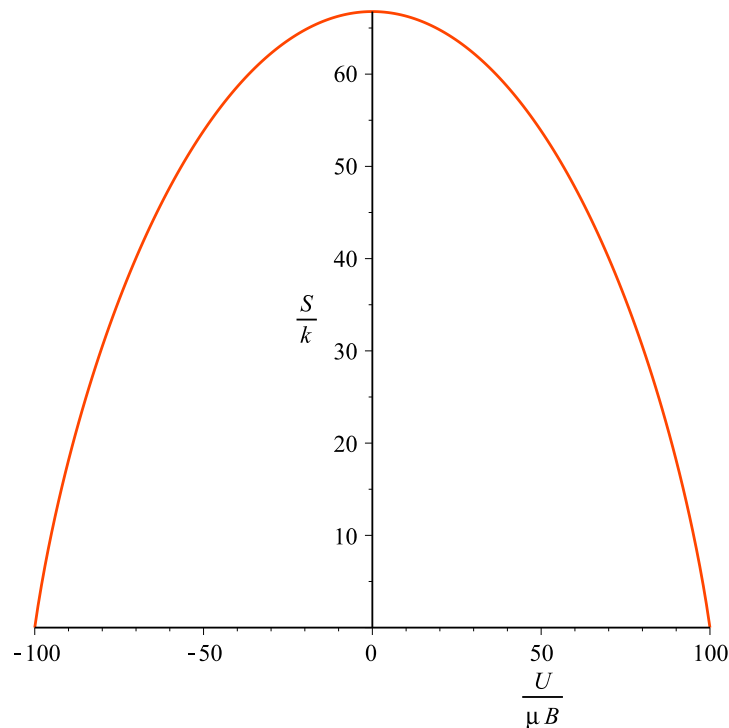
$$(3) \quad \Omega = \binom{N}{N_{\uparrow}} = \frac{N!}{N_{\uparrow}! (N - N_{\uparrow})!}$$

For small systems, we can find the entropy directly as

$$(4) \quad \frac{S}{k} = \ln \Omega$$

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

$$(5) \quad \frac{1}{T} = \frac{\partial S}{\partial U}$$

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 S by taking finite differences. Thus for a given value of N_{\uparrow} we can estimate the temperature as

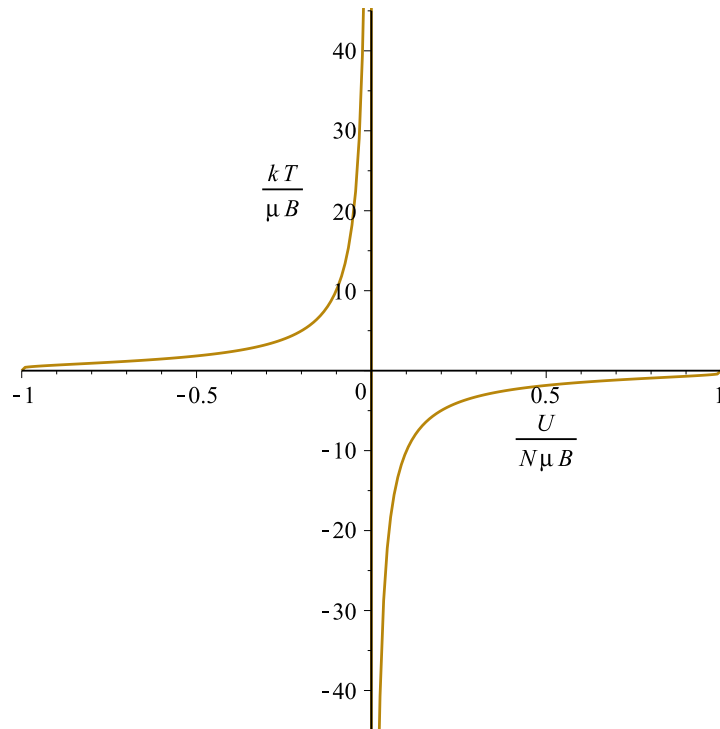
$$(6) \quad T(N_{\uparrow}) = \frac{\Delta U}{\Delta S}$$

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

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

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

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

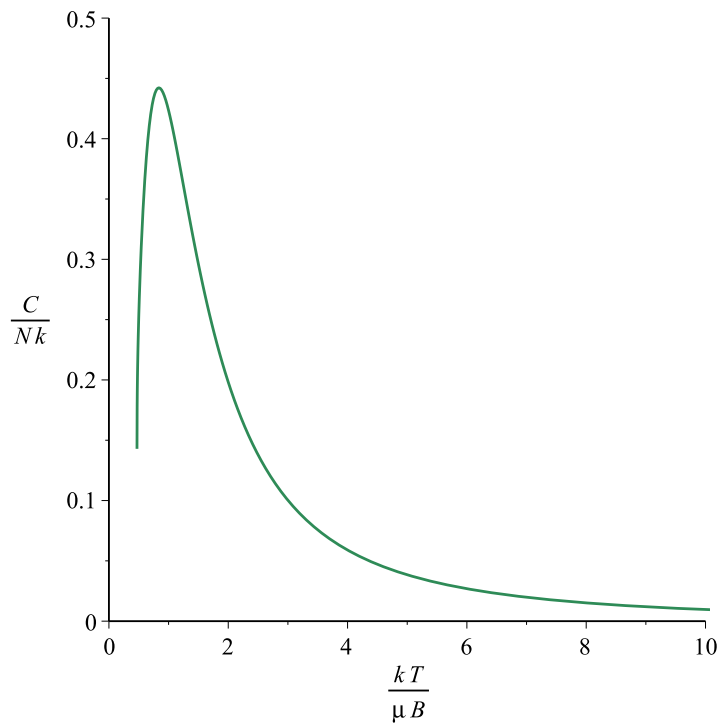
$$(9) \quad C = \frac{\Delta U}{\Delta T}$$

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

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

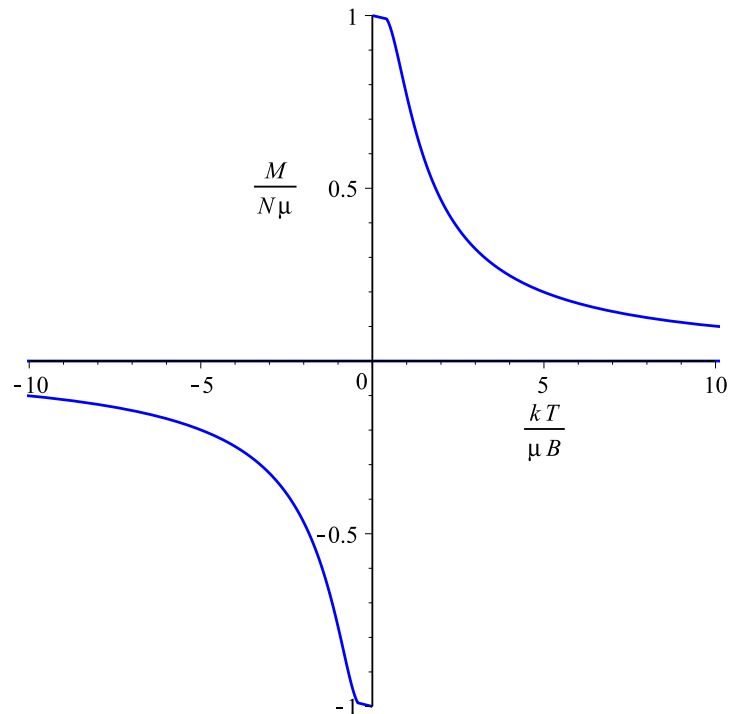
$$(11) \quad C(98) = 0.310Nk$$

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 $M \rightarrow 0$. 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 $T \rightarrow 0$ from the negative side.

PINGBACKS

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