TWO-STATE PARAMAGNET: AN EXPERIMENT WITH DPPH

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As an example of the formulas we obtained for the two-state paramagnet we can look at the experiment described in Schroeder dealing with the organic molecule DPPH, which is a real-life paramagnet with two spin states. The magnetization is given by

\[ M = N \mu \tanh \frac{\mu B}{kT} \]  

(1)

where in this example, the magnetic moment \( \mu \) is equal to the Bohr magneton \( \mu_B = \frac{e\hbar}{4\pi m_e} = 9.274 \times 10^{-24} \text{ J T}^{-1} \). Since the \( \tanh \) function has a maximum value of +1 which is reached asymptotically as its argument goes to +\( \infty \), the maximum magnetization is reached in the limit of very high applied field \( B \) and/or very low temperature \( T \).

For an applied field of 2.06 T and a temperature of 2.2 K, the fractional magnetization is

\[ \frac{M}{N\mu} = \tanh \left( \frac{9.274 \times 10^{-24}}{1.38 \times 10^{-23}} \right) \left( \frac{2.06}{2.2} \right) = 0.558 \]  

(2)

The magnetization can also be written as

\[ M = \mu \left( N_\uparrow - N_\downarrow \right) = \mu \left( N_\uparrow - (N - N_\uparrow) \right) = \mu \left( 2N_\uparrow - N \right) \]  

(3)

so

\[ \frac{M}{N\mu} = 2 \frac{N_\uparrow}{N} - 1 \]  

(4)

\[ n \equiv \frac{N_\uparrow}{N} = \frac{1}{2} \left( 1 + \tanh \frac{\mu B}{kT} \right) \]  

(5)

The entropy is
\[
S = N \ln N - N_\uparrow \ln N_\uparrow - (N - N_\uparrow) \ln (N - N_\uparrow) \tag{6}
\]
\[
= N \left[ \ln N - n (\ln N + \ln n) - (1 - n) (\ln N + \ln (1 - n)) \right] \tag{7}
\]
\[
= -N \left[ n \ln n + (1 - n) \ln (1 - n) \right] \tag{8}
\]

The maximum entropy occurs at \( n = \frac{1}{2} \) and is

\[
\frac{S_{\text{max}}}{kN} = \ln 2 = 0.693 \tag{9}
\]

If we plug 2 into 5 we get

\[
n = \frac{1}{2} (1 + 0.558) = 0.779 \tag{10}
\]

The fractional entropy is therefore

\[
\frac{S}{S_{\text{max}}} = -\frac{0.779 \ln 0.779 + 0.221 \ln 0.221}{0.693} = 0.762 \tag{11}
\]

The energy is

\[
U = \mu B (N_\downarrow - N_\uparrow) = \mu B (N - 2N_\uparrow) = \mu BN (1 - 2n) \tag{12}
\]

which is maximum when \( n = 0 \) and has value \( U_{\text{max}} = \mu BN \). The fractional energy in the above experiment is

\[
\frac{U}{U_{\text{max}}} = \frac{1 - 2 \times 0.779}{1} = -0.588 \tag{13}
\]

To achieve 99% magnetization, we would need

\[
\frac{M}{N \mu} = \tanh \frac{\mu B}{kT} = 0.99 \tag{14}
\]

\[
\frac{\mu B}{kT} = \tanh^{-1} 0.99 = 2.647 \tag{15}
\]

\[
\frac{B}{T} = 3.938 \text{ T K}^{-1} \tag{16}
\]

Thus with a magnetic field of 2.06 T, the temperature would need to be 0.523 K, or, conversely, if the temperature is held at 2.2 K, the field would need to be 8.66 T.