Physics 112 — Solution Set #4 — Winter 2000

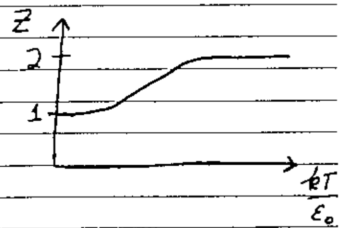
1. RB Chapter 5, problem 1

(a) The partition function is

$$Z = \sum_r e^{-E_r/kT}$$

In this problem, there are two energy levels: 0 and ε_0. Thus,

$$\boxed{Z = 1 + e^{-\varepsilon_0/kT}}$$



(b) The mean value of the energy is

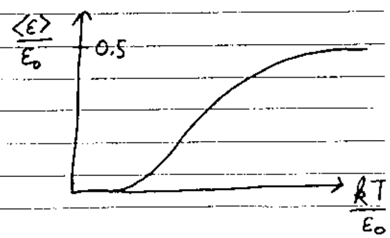
$$\langle \varepsilon \rangle = \frac{\sum_r \varepsilon_r e^{-E_r/kT}}{Z}$$

Thus,

$$\langle \varepsilon \rangle = \frac{\varepsilon_0 e^{-\varepsilon_0/kT}}{1 + e^{-\varepsilon_0/kT}}$$

Multiplying the numerator and denominator by $e^{\varepsilon_0/kT}$, we can rewrite $\langle \varepsilon \rangle$ as follows

$$\boxed{\langle \varepsilon \rangle = \frac{\varepsilon_0}{e^{\varepsilon_0/kT} + 1}}$$



(c) The heat capacity is

$$\boxed{C(T) = \frac{\partial \langle \varepsilon \rangle}{\partial T} = k\left(\frac{\varepsilon_0}{kT}\right)^2 \frac{e^{\varepsilon_0/kT}}{(e^{\varepsilon_0/kT} + 1)^2}}$$

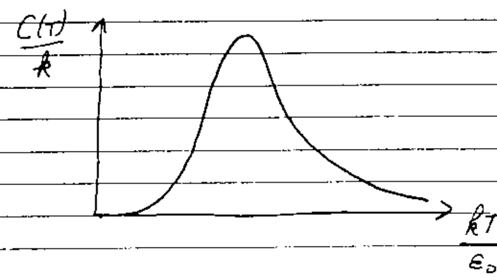
To graph this function, we note that as $T \to 0$, $e^{\varepsilon_0/kT} \gg 1$. Thus, we can drop the factor of $+1$ in the denominator, obtaining:

$$C(T) \simeq k\left(\frac{\varepsilon_0}{kT}\right) e^{-\varepsilon_0/kT}, \qquad T \to 0$$

which is exponentially suppressed. As $T \to \infty$, $e^{\varepsilon_0/kT} = 1 + O\left(\frac{\varepsilon_0}{kT}\right)$. Thus,

$$C(T) \simeq \frac{k}{4}\left(\frac{\varepsilon_0}{kT}\right)^2, \qquad T \to \infty$$

which vanishes like a power. Clearly, $C(T) > 0$ for all T, so $C(T)$ must reach a maximum somewhere in the middle. The graph then looks like



(d) To compute the entropy, use the relation

$$S = \frac{\langle \varepsilon \rangle}{T} + k \ln Z$$

Using the results of parts (a) and (b),

$$\boxed{S = \frac{\varepsilon_0}{T}\frac{1}{e^{\varepsilon_0/kT}+1} + k\ln\left(1+e^{-\varepsilon_0/kT}\right)}$$

Look at the cases of small and large T.
As $T \to 0$,

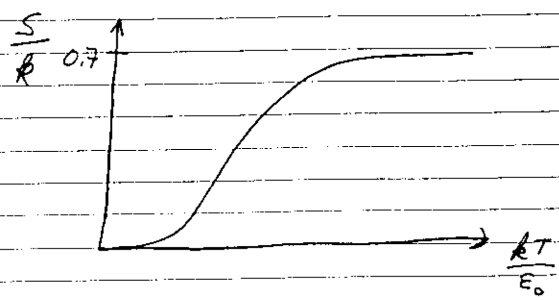
$$\ln(1+e^{-\varepsilon_0/kT}) \simeq e^{-\varepsilon_0/kT}$$

since $\ln(1+z) \simeq z$ for $|z| \ll 1$. Similarly, we can drop the $+1$ in the denominator of the first term. Thus,

$$S \simeq k\left(\frac{\varepsilon_0}{kT}+1\right)e^{-\varepsilon_0/kT}$$

$$\simeq \frac{\varepsilon_0}{T}e^{-\varepsilon_0/kT} \qquad \text{as } T \to 0$$

As $T \to \infty$, $S \to k\ln 2$. Thus, the graph looks like



noting that $\ln 2 = 0.6931$

② RB Chapter 5, problem 2

The three energy levels are:

	energy	S_z
spin "up"	ε_0	$\hbar$
spin "sideways"	0	0
spin "down"	ε_0	$-\hbar$

Thus, the partition function is

$$Z = 1 + 2e^{-\varepsilon_0/kT}$$

since the level with energy ε_0 is doubly degenerate.

(a) $$P_{up} = \frac{e^{-\varepsilon_0/kT}}{Z} = \frac{e^{-\varepsilon_0/kT}}{1+2e^{-\varepsilon_0/kT}}$$

which we can rewrite as

$$P_{up} = \frac{1}{2+e^{\varepsilon_0/kT}}$$

In order that $P_{up} = \frac{1}{3}$, we must have $e^{\varepsilon_0/kT} = 1$ or $\frac{\varepsilon_0}{kT} = 0$.
This corresponds to the limit of $T \to \infty$.

(b) Following the same steps as in the previous problem,

$$\langle \varepsilon \rangle = \frac{1}{Z}2\varepsilon_0 e^{-\varepsilon_0/kT} = 2\varepsilon_0 P_{up}$$

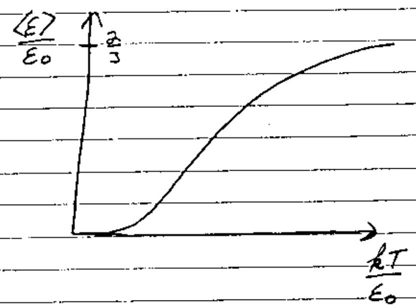
which makes sense since $P_{up} = P_{down}$. From part (a),

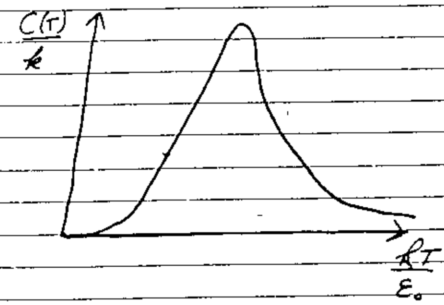
$$\langle \varepsilon \rangle = \frac{2\varepsilon_0}{2 + e^{\varepsilon_0/kT}}$$

The heat capacity is

$$C(T) = \frac{d\langle \varepsilon \rangle}{dT} = 2k\left(\frac{\varepsilon_0}{kT}\right)^2 \frac{e^{\varepsilon_0/kT}}{(2+e^{\varepsilon_0/kT})^2}$$

The graphs are similar to those of problem 2. Note that as $T \to \infty$, $\frac{\langle \varepsilon \rangle}{\varepsilon_0} \to \frac{2}{3}$. Thus,





(c) We can easily work out:

$$\langle S_z \rangle = (+\hbar) P_{up} + (0) P_{sideways} + (-\hbar) P_{down}$$

But $P_{up} = P_{down}$. Thus,

$$\langle S_z \rangle = 0.$$

This is to be expected since spin up and spin down occur with equal probability and thus average out to zero.

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③ RB Chapter 5, problem 5

(a) First note that for the case of $N=1$, the energy levels are:

state index j	orientation of moment relative to $\vec{B}$	system energy E_j
1	parallel	$-m_B B$
2	anti-parallel	$+m_B B$

as shown in Table 5.1 of RB (p95). Thus,

$$Z_1 = e^{m_B B/kT} + e^{-m_B B/kT} = 2\cosh\left(\frac{m_B B}{kT}\right)$$

as obtained in eq. (5.14).

In the case of $N=2$ we have four possible states:

state index j	$\varepsilon(1)$	$\varepsilon(2)$	E_j
1	$-m_B B$	$-m_B B$	$-2m_B B$
2	$+m_B B$	$-m_B B$	0
3	$-m_B B$	$+m_B B$	0
4	$+m_B B$	$+m_B B$	$+2m_B B$

where $E_j = \varepsilon(1) + \varepsilon(2)$ is the sum of the single particle energies. Hence,

$$Z_2 = \sum_{j=1}^{4} e^{-E_j/kT} = e^{2m_B B/kT} + 2 + e^{-2m_B B/kT}$$
$$= \left(e^{m_B B/kT} + e^{-m_B B/kT}\right)^2$$
$$= Z_1^2$$

(b) For the general case of N spins,

$$Z_N = Z_1^N$$

Thus, $\ln Z_N = N \ln Z_1$.

We can compute $\langle E \rangle$ from the formula [RB eq (5.16)]

$$\langle E \rangle = kT^2 \frac{1}{Z_N}\frac{\partial Z_N}{\partial T} = kT^2 \frac{\partial}{\partial T}\ln Z_N$$

$$= kT^2 N \frac{\partial}{\partial T}\ln Z_1$$

$$= kT^2 N \frac{1}{Z_1}\frac{\partial Z_1}{\partial T}$$

Using $Z_1 = 2\cosh\left(\frac{m_B B}{kT}\right)$,

$$\langle E \rangle = -N m_B B \tanh\left(\frac{m_B B}{kT}\right)$$

Likewise, the mean value of the magnetic moment along $\vec{B}$ is given by [RB eq S.20]

$$\langle \text{magnetic moment along } \vec{B} \rangle = kT \frac{\partial}{\partial B}\ln Z_N$$

$$= NkT \frac{\partial}{\partial B}\ln Z_1$$

$$= NkT \frac{1}{Z_1}\frac{\partial Z_1}{\partial B}$$

Evaluating the derivative, one gets

$$\langle \text{total magnetic moment along } \vec{B} \rangle = N m_B \tanh\left(\frac{m_B B}{kT}\right).$$

(c) Consider

$$\langle E \rangle = \frac{1}{Z}\sum_j E_j e^{-E_j/kT}$$

$$\frac{\partial \langle E \rangle}{\partial T} = \frac{\partial}{\partial T}\left(\frac{1}{Z}\right)\sum_j E_j e^{-E_j/kT} + \frac{1}{Z}\sum_j E_j \frac{E_j}{kT^2} e^{-E_j/kT}$$

Using $\frac{\partial}{\partial T}\left(\frac{1}{Z}\right) = -\frac{1}{Z^2}\frac{\partial Z}{\partial T} = -\frac{1}{Z}\frac{\langle E \rangle}{kT^2}$

where the last step follows from RB eq (5.16),

$$\frac{\partial \langle E \rangle}{\partial T} = -\frac{1}{kT^2}\langle E \rangle^2 + \frac{1}{kT^2}\langle E^2 \rangle$$

Since $\langle E^2 \rangle = \frac{1}{Z}\sum_j E_j^2 e^{-E_j/kT}$

Finally, recall that

$$\langle (E - \langle E \rangle)^2 \rangle = \langle E^2 \rangle - 2\langle E \langle E \rangle \rangle + \langle E \rangle^2$$

$$= \langle E^2 \rangle - 2\langle E \rangle^2 + \langle E \rangle^2$$

$$= \langle E^2 \rangle - \langle E \rangle^2$$

Thus,

$$\boxed{\langle (E-\langle E\rangle)^2\rangle = kT^2 \frac{\partial \langle E\rangle}{\partial T}}$$

For the spin system,

$$\langle E\rangle = -N m_B B \tanh\left(\frac{m_B B}{kT}\right)$$

$$\frac{\partial \langle E\rangle}{\partial T} = \frac{N(m_B B)^2}{kT^2}\,\mathrm{sech}^2\left(\frac{m_B B}{kT}\right)$$

Using the above formula for $(\Delta E)^2 \equiv \langle (E-\langle E\rangle)^2\rangle$,

$$\Delta E = \sqrt{N}\, m_B B\, \mathrm{sech}\left(\frac{m_B B}{kT}\right)$$

and so,

$$\frac{\Delta E}{|\langle E\rangle|} = \frac{1}{\sqrt{N}}\,\frac{1}{\sinh\left(\frac{m_B B}{kT}\right)}$$

In particular, we note that provided $\sinh\left(\frac{m_B B}{kT}\right)$ is of order unity,

$$\frac{\Delta E}{|\langle E\rangle|} = O\left(\frac{1}{\sqrt{N}}\right)$$

(d) When $N \sim O(N_A)$ where $N_A = 6.022\times 10^{23}$ is Avagadro's number, we see that the fractional uncertainty in the energy is incredibly small. A similar computation would also show that the fractional uncertainty in the total magnetic moment along $\vec{B}$ is also of $O\left(\frac{1}{\sqrt{N}}\right)$ and is likewise negligible.

(e) The specific heat is given by

$$C(T) = \frac{\partial \langle E\rangle}{\partial T} = \frac{1}{kT^2}(\Delta E)^2$$

using the results of part (c). This is a general result for the canonical probability distribution in general.

Clearly, $(\Delta E)^2 \geq 0$. Hence we conclude that

$$C(T) \geq 0.$$

Note that one expects that $E \neq \langle E\rangle$ (there is always some thermal fluctuation), in which case $(\Delta E)^2$ is strictly positive. Then, we can conclude that $C(T) > 0$.

④ RB Chapter 5, problem 7

(a) The partition function is given by [RB eq. (5.22)]

$$Z = \int_0^\infty e^{-E/kT} D(E)\,dE$$

Assuming that $D(E) = g(N,V)\,E^{\frac{3N}{2}-1}$,

$$Z = g(N,V)\int_0^\infty e^{-E/kT} E^{\frac{3N}{2}-1}\,dE$$

Let $x = \frac{E}{kT}$. Then,

$$Z = g(N,V)(kT)^{\frac{3N}{2}} \int_0^\infty e^{-x} x^{\frac{3N}{2}-1}\,dx$$

$$= g(N,V)(kT)^{\frac{3N}{2}}\,\Gamma\!\left(\frac{3N}{2}\right)$$

where Γ is the well-known gamma function. If N is even, we can use $\Gamma(n+1) = n!$ to write:

$$Z = g(N,V)(kT)^{\frac{3N}{2}}\left(\frac{3N}{2}-1\right)!$$

(b) According to RB eq. (5.24), we can write

$$Z = e^{-\langle E\rangle/kT} D(\langle E\rangle)\,\delta E$$

which defines δE. To evaluate this, we need to work out $\langle E\rangle$

$$\langle E\rangle = \frac{1}{Z}\int_0^\infty E\, e^{-E/kT} D(E)\,dE$$

$$= \frac{g(N,V)}{Z}\int_0^\infty e^{-E/kT} E^{\frac{3N}{2}}\,dE$$

$$= \frac{g(N,V)(kT)^{\frac{3N}{2}+1}}{Z}\left(\frac{3N}{2}\right)!$$

Inserting $Z = g(N,V)(kT)^{\frac{3N}{2}}\left(\frac{3N}{2}-1\right)!$ from part (a) yields

$$\boxed{\langle E\rangle = \frac{3}{2}NkT}$$

We could have also derived the same result from

$$\langle E\rangle = kT^2 \frac{\partial}{\partial T}\ln Z$$

Thus,

$$\delta E = \frac{Z}{e^{-\langle E\rangle/kT} D(\langle E\rangle)}$$

$$= \frac{g(N,V)(kT)^{\frac{3N}{2}}\left(\frac{3N}{2}-1\right)!}{e^{-\frac{3}{2}N} g(N,V)\left(\frac{3}{2}NkT\right)^{\frac{3N}{2}-1}}$$

$$= \frac{\left(\frac{3N}{2}-1\right)!\;kT}{e^{-\frac{3}{2}N}\left(\frac{3N}{2}\right)^{\frac{3N}{2}-1}}$$

which can be rewritten as

$$\delta E = \frac{\left(\frac{3N}{2}\right)!\, kT}{e^{-\frac{3}{2}N}\left(\frac{3N}{2}\right)^{\frac{3N}{2}}}$$

Finally, using Stirling's approximation,

$$n! \simeq \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \quad , \quad n \gg 1$$

we can write:

$$\delta E \simeq \frac{\sqrt{2\pi}\left(\frac{3N}{2}\right)^{\frac{3N}{2}+\frac{1}{2}} e^{-\frac{3}{2}N}\, kT}{e^{-\frac{3}{2}N}\left(\frac{3N}{2}\right)^{\frac{3N}{2}}}$$

or $$\boxed{\delta E \simeq \sqrt{3\pi N}\, kT}$$

(c) In part (b), we have already worked out $\langle E \rangle = \frac{3}{2}NkT$.
Thus,

$$\boxed{\frac{\delta E}{\langle E \rangle} \simeq \frac{2}{3}\sqrt{\frac{3\pi}{N}}}$$

In particular, we note that $\frac{\delta E}{\langle E \rangle} = O\left(\frac{1}{\sqrt{N}}\right)$

and again we find that the fractional uncertainty in the energy is completely negligible when N is a macroscopic number, say $N = O(N_A)$.