Physics 112   Solution Set #4   Winter 2000

(c) The heat capacity is

\[ C(T) = \frac{\partial \langle E \rangle}{\partial T} = \frac{\partial}{\partial T} \left( \frac{e^{E_0/RT}}{1 + e^{E_0/RT}} \right) \]

To graph this function, we note that as \( T \to 0 \), \( e^{E_0/RT} \to 0 \). Thus, we can drop the factor of \( 1 \) in the denominator, obtaining:

\[ C(T) = N \left( \frac{E_0}{RT} \right) e^{-E_0/RT} \quad T \to 0 \]

which is exponentially suppressed. As \( T \to \infty \), \( e^{E_0/RT} = 1 + \frac{E_0}{RT} \).

Thus,

\[ C(T) \approx \frac{\langle E_0 \rangle}{4 RT} \quad T \to \infty \]

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

(c) To compute the entropy, we use the relation

\[ S = \frac{\langle E \rangle + k \ln Z}{T} \]
Using the results of parts (a) and (b),

\[ S = \frac{E_0}{T} \ln \left( 1 + e^{-\frac{E_0}{kT}} \right) . \]

Look at the cases of small and large \( T \).

As \( T \to 0 \),

\[ \ln \left( 1 + e^{-\frac{E_0}{kT}} \right) \approx e^{-\frac{E_0}{kT}} \]

since \( \ln (1+e) \approx e \) for \( 1 \ll e \). Similarly, we can drop the \( -1 \) in the denominator of the first term. Thus,

\[ S = \frac{k}{kT} e^{-\frac{E_0}{kT}} \]

\[ = \frac{E_0 e^{-\frac{E_0}{kT}}}{kT} \quad \text{as} \quad T \to 0 \]

As \( T \to \infty \), \( S \to \ln 2 \). This is graphed below.

\[ S \] \hspace{3cm} \[ \frac{k}{E_0} \]

\[ \frac{0.7}{0.7} \]

noting that \( \ln 2 = 0.6931 \).

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(3)
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4. RB Chapter 5, Problem 2

The three energy levels are:

<table>
<thead>
<tr>
<th>Energy Level</th>
<th>energy</th>
<th>( e_0 )</th>
<th>( \frac{\text{eq}}{kT} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>spin &quot;up&quot;</td>
<td></td>
<td>( e_0 )</td>
<td>-</td>
</tr>
<tr>
<td>spin &quot;down&quot;</td>
<td></td>
<td>( e_0 )</td>
<td>-</td>
</tr>
<tr>
<td>spin &quot;labeled&quot;</td>
<td></td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Thus, the partition function is

\[ Z = 1 + 2e^{-\frac{E_0}{kT}} \]

Since the level with energy \( e_0 \) is doubly degenerate,

(a) \[ P_{up} = \frac{e^{-\frac{E_0}{kT}}}{Z} = \frac{e^{-\frac{E_0}{kT}}}{1 + 2e^{-\frac{E_0}{kT}}} \]

which we can rewrite as

\[ P_{up} = \frac{1}{2 + e^{-\frac{E_0}{kT}}} \]

In order that \( P_{up} = \frac{1}{2} \), we must have \( e^{-\frac{E_0}{kT}} = 1 \) or \( E_0 = 0 \).

This corresponds to the limit of \( T \to \infty \).

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

\[ \langle E \rangle = \frac{1}{2} 2e_0 e^{-\frac{E_0}{kT}} = 2e_0 P_{up} \]

which makes sense since \( P_{up} = P_{down} \). From part (a),
\[
\langle E \rangle = \frac{2E_0}{2 + e^{E_0/kT}}
\]

The least capacity is

\[
C(T) = \frac{d\langle E \rangle}{dT} = \frac{2E_0^2}{(2 + e^{E_0/kT})^2} \frac{e^{E_0/kT}}{kT}
\]


The graphs are similar to those of problem 1. Note that as \( T \to \infty \),

\[
\frac{\langle E \rangle}{E_0} \to \frac{2}{3}
\]

Thus,

\[
C(T) \to \frac{2E_0^2}{3}\]

(c) We can easily work out:

\[
\langle S_z \rangle = (\pm \hbar) \rho_{up} + (0) \rho_{down} + (-\hbar) \rho_{down}
\]

But \( \rho_{up} = \rho_{down} \). 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.

3. RB Chapter 5, problem 5

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

<table>
<thead>
<tr>
<th>State index</th>
<th>Orientation of electron relative to ( B )</th>
<th>Energy ( E_z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>parallel</td>
<td>(-m_0B)</td>
</tr>
<tr>
<td>2</td>
<td>anti-parallel</td>
<td>( m_0B)</td>
</tr>
</tbody>
</table>

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

\[
E_z = e^{m_0B/kT} + e^{-m_0B/kT} = 2 \cosh \left( \frac{m_0B}{kT} \right)
\]

as obtained in eq. (5.14).

In the case of \( N=2 \) we have four possible states:

<table>
<thead>
<tr>
<th>State index</th>
<th>( E(1) )</th>
<th>( E(2) )</th>
<th>( E_z )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(-m_0B)</td>
<td>(-m_0B)</td>
<td>(-2m_0B)</td>
</tr>
<tr>
<td>2</td>
<td>(+m_0B)</td>
<td>(-m_0B)</td>
<td>( 0 )</td>
</tr>
<tr>
<td>3</td>
<td>(-m_0B)</td>
<td>(+m_0B)</td>
<td>( 0 )</td>
</tr>
<tr>
<td>4</td>
<td>(+m_0B)</td>
<td>(+m_0B)</td>
<td>(+2m_0B)</td>
</tr>
</tbody>
</table>

where \( E_z = E(1) + E(2) \) is the sum of the single particle energies.

Hence,

\[
Z_1 = \sum_{i=1}^{4} e^{-E(i)/kT} = e^{3m_0B/kT} + 2 + e^{-3m_0B/kT}
\]

\[
= \left( e^{m_0B/kT} + e^{-m_0B/kT} \right)^2
\]

\[
= Z_1^2
\]
(b) For the general case of $N$ spins,

$$Z_N = Z_2^N$$

Thus, $\ln Z_N = N \ln Z_2$.

We can compute $\langle E \rangle$ from the formula [RB eq. (5.14)]

$$\langle E \rangle = kT \frac{\partial}{\partial T} \ln Z_N = kT \frac{\partial}{\partial T} \ln Z_2$$

$$= kT^2 N \frac{\partial}{\partial T} \ln Z_2$$

Using $Z_2 = \frac{1}{2} \tanh \left( \frac{\mu B}{kT} \right)$,

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

Similarly, the mean value of the magnetic moment along $\mathbf{B}$ is given by [RB eq. 5.20].

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

$$= N k T \frac{\partial}{\partial \mathbf{B}} \ln Z_2$$

$$= N k T \frac{1}{2} \frac{\partial Z_2}{\partial \mathbf{B}}$$

Evaluating the derivative, one gets

$$\langle \text{magnetic moment along } \mathbf{B} \rangle = \frac{N k}{2} \frac{\partial}{\partial \mathbf{B}} \tanh \left( \frac{\mu B}{kT} \right)$$

(c) Consider

$$\langle E \rangle = \frac{1}{Z} \sum_1^N E_2 \exp \left( -\frac{E_2}{kT} \right)$$

$$\frac{\partial \langle E \rangle}{\partial T} = \frac{1}{Z} \sum_1^N E_2 \exp \left( -\frac{E_2}{kT} \right) + \frac{1}{2} \sum_1^N E_2 \frac{\partial}{\partial T} \left( \exp \left( -\frac{E_2}{kT} \right) \right)$$

Using

$$\frac{\partial \left( \exp \left( -\frac{E_2}{kT} \right) \right)}{\partial T} = -\frac{1}{2} \frac{\partial Z}{\partial T} = -\frac{1}{Z} \frac{\partial \langle E \rangle}{\partial T}$$

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

$$\langle E^2 \rangle = \frac{1}{Z} \sum_1^N E_2^2 \exp \left( -\frac{E_2}{kT} \right)$$

Finally, recall that

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

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

$$= \langle E^2 \rangle - \langle E \rangle^2$$
Thus,
\[
\langle (E - \langle E \rangle)^2 \rangle = kT \frac{\partial^2 \langle E \rangle}{\partial T^2}
\]

For the spin system,
\[
\langle E \rangle = -N m g B \text{log} \left( \frac{m_B}{kT} \right)
\]

\[
\frac{\partial \langle E \rangle}{\partial T} = \frac{N m^2 g B^2}{kT} \text{sech}^2 \left( \frac{m_B}{kT} \right)
\]

Using the above formula for \( (\Delta E)^2 = \langle (E - \langle E \rangle)^2 \rangle \),
\[
\Delta E = \sqrt{N} m g B \text{sech} \left( \frac{m_B}{kT} \right)
\]

and so,
\[
\frac{\Delta E}{|\langle E \rangle|} = \frac{1}{\sqrt{N}} \frac{1}{\text{sech} \left( \frac{m_B}{kT} \right)}
\]

In particular, we note that provided \( \text{sech}(\frac{m_B}{kT}) \) is of order unity,
\[
\frac{\Delta E}{|\langle E \rangle|} = O \left( \frac{1}{\sqrt{N}} \right)
\]

(\(d\)) When \( N = O(N_a) \) where \( N_a = 6.022 \times 10^{23} \) is Avogadro'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 \( B \) is also of \( O \left( \frac{1}{\sqrt{N}} \right) \) and is likewise negligible.
(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 \( D(E) = g(N,V) \frac{e^{-E/kT}}{E^{3N-1}} \),

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

Let \( x = E \). Then,

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

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

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

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

(b) According to RB Eq. (5.21), we can write

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

which defines \( \delta E \). To evaluate this, we need to work out \( \langle E \rangle \).

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

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

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

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

\[ \langle E \rangle = \frac{3NkT}{2} \left( \frac{3N}{2} \right)! \]

We could have also derived the same result from

\[ \langle E \rangle = \frac{1}{Z^2} \frac{\partial}{\partial T} \ln Z \]

Thus,

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

\[ = \frac{g(N,V) (kT)^{\frac{3N}{2}} \left( \frac{3N}{2} \right)! \left( \frac{3N}{2} \right)!}{e^{-\langle E \rangle/kT} D(\langle E \rangle)} \]

\[ = \frac{\left( \frac{3N}{2} - 1 \right)! \frac{kT}{(\frac{3N}{2})^{\frac{3N}{2}+1}}}{e^{-\langle E \rangle/kT} D(\langle E \rangle)} \]

\[ = \frac{\left( \frac{3N}{2} - 1 \right)! \frac{kT}{(\frac{3N}{2})^{\frac{3N}{2}+1}}}{e^{-\langle E \rangle/kT} D(\langle E \rangle)} \]
which can be rewritten as

$$\delta E = \frac{(2N)!}{e^{\frac{2N}{2}}} kT$$

Finally, using Stirling's approximation,

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

we can write:

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

or

$$\delta E = \sqrt{3\pi N} kT$$

(c) In part (b), we have already worked out

$$\langle E \rangle = \frac{3}{2} N kT$$

Thus,

$$\delta E = 2 \frac{\sqrt{\pi}}{3 \sqrt{N}}$$

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 $N = 0(1/A)$. 