# Problem Sheet 2

Magnets and Oscillators

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# Magnets and oscillators

## 2.1

**(i)** The energy levels are given by:

$$E_\pm = \pm \mu_B B \tag{1}$$

The single particle partition function is:

$$Z_1 = e^{-\beta \mu_B B} + e^{\beta \mu_B B} = 2 \cosh\left(\beta \mu_B B\right) \tag{2}$$

**(ii)** The partition function for $N$ non-interacting particles is:

$$Z = Z_1^N = [2 \cosh\left(\beta \mu_B B\right)]^N \tag{3}$$

so that the internal energy is:

$$
\begin{aligned}
U &= -\frac{\partial \ln Z}{\partial \beta} \\
&= -N \frac{\partial \ln\left[2 \cosh\left(\beta \mu_B B\right)\right]}{\partial \beta} \\
&= -N \mu_B B \tanh\left(\beta \mu_B B\right)
\end{aligned}
\tag{4}
$$

The heat capacity is:

$$C_B = \left(\frac{\partial U}{\partial T}\right)_B = N k_B \left(\frac{\theta}{T}\right)^2 \frac{1}{\cosh^2\left(\theta/T\right)} \tag{5}$$

where we identify the temperature scale:

$$\theta \equiv \frac{\mu_B B}{k_B} \tag{6}$$

The maximum of $C_B$ can be derived by setting the derivative to zero. Denoting $x = \theta/T$, we have:

$$
\begin{aligned}
\frac{\partial C_B}{\partial x} &\propto -2x^2 \frac{\sinh x}{\cosh^3 x} + 2x \frac{1}{\cosh^2 x} \\
&= 2x \frac{1 - x \tanh x}{\cosh^2 x}
\end{aligned}
\tag{7}
$$

Thus, the maximum of $C_B$ occurs at $x = \tanh x$, which is approximately $x = 1.20$. Therefore, the maximum of $C_B$ occurs at:

$$T_{\text{peak}} = \frac{\theta}{1.20} = 0.83 \frac{\mu_B B}{k_B} \tag{8}$$

(iii)   With $B = 2\,\text{T}$ and $\mu_B = 9.27 \times 10^{-24}\,\text{J/T}$, we have:

$$T_{\text{peak}} = 1.119\,\text{K} \tag{9}$$

at which the heat capacity of the system is significant.

(iv)   At high $T$, we have $\theta/T \ll 1$, so that $\cosh(\theta/T) \approx 1$ and $C_B \propto T^{-2}$. At low $T$, we have $\theta/T \gg 1$, so that:

$$C_B \propto \frac{1}{T^2} \frac{e^{\theta/T}}{e^{2\theta/T}} \propto \frac{e^{-\theta/T}}{T^2} \tag{10}$$

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## 2.2

The partition function for a single particle in a harmonic oscillator potential is:

$$Z_1 = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+1/2)} = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} = \frac{1}{2\sinh(\beta\hbar\omega/2)} \tag{11}$$

The partition function for $N$ non-interacting particles is:

$$Z = Z_1^N = \frac{1}{[2\sinh(\beta\hbar\omega/2)]^N} \tag{12}$$

The internal energy is:

$$U = -\left(\frac{\partial \ln Z}{\partial \beta}\right)_V$$
$$= \frac{N\hbar\omega}{2} + \frac{N\hbar\omega}{\exp(\beta\hbar\omega) - 1} \tag{13}$$

so that the specific heat is:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = N k_B \left(\frac{\hbar\omega}{k_B T}\right)^2 \frac{\exp\left(\beta\hbar\omega\right)}{[\exp\left(\beta\hbar\omega\right) - 1]^2} = N k_B \left[\frac{\beta\hbar\omega/2}{\sinh\left(\beta\hbar\omega/2\right)}\right]^2 \tag{14}$$

In high temperature limit, we have $\beta\hbar\omega \ll 1$, so that $C_V \to N k_B$. In low temperature limit, we have $\beta\hbar\omega \gg 1$, so that $C_V \to 0$.

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## 2.3

The free energy of a single particle in a harmonic oscillator potential is:

$$F_1 = -k_B T \ln Z_1 = -k_B T \ln \left[\frac{1}{2\sinh\left(\beta\hbar\omega/2\right)}\right] \tag{15}$$

so that the entropy (scaled by $k_B$) is:

$$\frac{S_1}{k_B} = -\frac{1}{k_B}\left(\frac{\partial F_1}{\partial T}\right)_V = \ln\left[\frac{1}{2\sinh\left(\theta/T\right)}\right] + \frac{\theta}{T}\frac{\cosh\left(\theta/T\right)}{\sinh\left(\theta/T\right)} \tag{16}$$

where we define the temperature scale $\theta \equiv \hbar\omega/2k_B$.

We require the internal energy of system, defined as:

$$U = -\left(\frac{\partial \ln Z_1}{\partial \beta}\right)_V = \frac{\hbar\omega}{2} + \frac{\hbar\omega}{\exp\left(2\theta/T\right) - 1} \tag{17}$$

to equal $(m + 1/2)\hbar\omega$.

This puts a constraint on the temperature:

$$\frac{1}{\exp\left(2\theta/T\right) - 1} = m \tag{18}$$

or equivalently $e^{2\theta/T} = 1 + 1/m$.

Substituting this into the entropy expression, we have:

$$\begin{aligned}
\frac{S_1}{k_B} &= -\ln\left(\sqrt{1 + 1/m} - \frac{1}{\sqrt{1 + 1/m}}\right) + (1 + 2m)\ln\sqrt{1 + 1/m} \\
&= -\ln\left(\frac{1}{\sqrt{m^2 + m}}\right) + (1 + 2m)\ln\sqrt{1 + 1/m} \\
&= (m + 1)\ln\left(m + 1\right) - m\ln m
\end{aligned} \tag{19}$$

which is the desired result.

When $m \to 0$, we have $S_1 \to 0$. This means that the entropy is zero (which is an arbitrary reference value) when every particle is in the ground state.

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## 2.4

**(i)** The single particle partition function is:

$$
\begin{aligned}
Z_M &= \sum_{k=-J}^{J} \exp\left(\beta k g_J \mu_B B\right) \\
&= \sum_{k=-J}^{J} \exp\left(kC\right) \\
&= \frac{e^{-JC} - e^{(J+1)C}}{1 - e^C} \\
&= \frac{\sinh\left[(J + 1/2)C\right]}{\sinh\left(C/2\right)}
\end{aligned}
\tag{20}
$$

where $C \equiv g_J \mu_B B / k_B T$.

**(ii)** Consider the free energy for $\mathcal{N} = NV$ particles:

$$
F = \mathcal{N} F_1 = -\mathcal{N} k_B T \ln Z_M
\tag{21}
$$

The total magnetic moment is:

$$
m = -\mathcal{N} \left(\frac{\partial F_1}{\partial B}\right)_T
\tag{22}
$$

so that the magnetization is:

$$
\begin{aligned}
M &= \frac{m}{V} \\
&= -N \left( \frac{\partial F_1}{\partial B} \right)_T \\
&= -N \frac{g_J \mu_B}{k_B T} \left( \frac{\partial F_1}{\partial C} \right)_T \\
&= N g_J \mu_B \left[ \frac{J + 1/2}{\tanh\left[(J + 1/2)C\right]} - \frac{1/2}{\tanh\left(C/2\right)} \right] \\
&= N g_J \mu_B \frac{1}{C} \left[ \frac{(J + 1/2)C}{\tanh\left[(J + 1/2)C\right]} - \frac{C/2}{\tanh\left(C/2\right)} \right]
\end{aligned}
\tag{23}
$$

Thus, the susceptibility can be taken as:

$$
\begin{aligned}
\chi &= \frac{\mu_0 M}{B} \\
&= \frac{\mu_0 N g_J^2 \mu_B^2}{k_B T} \frac{1}{C^2} \left[ \frac{(J + 1/2)C}{\tanh\left[(J + 1/2)C\right]} - \frac{C/2}{\tanh\left(C/2\right)} \right] \\
&\approx \frac{\mu_0 N g_J^2 \mu_B^2}{k_B T} \frac{1}{C^2} \left( \frac{\left[(J + 1/2)C\right]^2}{3} - \frac{C^2/4}{3} \right) \\
&= \frac{\mu_0 N g_J^2 \mu_B^2}{3 k_B T} J(J + 1)
\end{aligned}
\tag{24}
$$

which reduces to the Curie law for $J = 1/2$.

**(iii)**   Define the partition function for a harmonic oscillator as:

$$
Z_{\text{SHO}}(\hbar\omega) = \frac{1}{2 \sinh\left(\beta\hbar\omega/2\right)}
\tag{25}
$$

We can check that $Z_M$ is a ratio of two partition functions:

$$
Z_M = \frac{Z_{\text{SHO}}(g_J \mu_B B)}{Z_{\text{SHO}}\left[(2J + 1)g_J \mu_B B\right]}
\tag{26}
$$

Consider the logarithm of $-Z_M$:

$$
-\ln Z_M = -\ln Z_{\text{SHO}}(g_J \mu_B B) + \ln Z_{\text{SHO}}\left[(2J + 1)g_J \mu_B B\right]
\tag{27}
$$

This means that the free energy is that of a harmonic oscillator with frequency $g_J \mu_B B$ minus that of a harmonic oscillator with frequency $(2J + 1)g_J \mu_B B$.

**(iv)**   Given the form of $Z_M$ as a ratio of harmonic oscillator partition functions, we can write the internal energy as:

$$
\begin{aligned}
U &= -\left(\frac{\partial \ln Z_M}{\partial \beta}\right)_V \\
&= -\left(\frac{\partial \ln Z_{\mathrm{SHO}}(g_J\mu_B B)}{\partial \beta}\right)_V + \left(\frac{\partial \ln Z_{\mathrm{SHO}}[(2J+1)g_J\mu_B B]}{\partial \beta}\right)_V \\
&= U_{\mathrm{SHO}}(g_J\mu_B B) - U_{\mathrm{SHO}}[(2J+1)g_J\mu_B B]
\end{aligned}
\tag{28}
$$

This implies that the heat capacity can be written as a difference of those for the two harmonic oscillators:

$$
\begin{aligned}
C_V &= \left(\frac{\partial U}{\partial T}\right)_V \\
&= C_{V,\mathrm{SHO}}(g_J\mu_B B) - C_{V,\mathrm{SHO}}[(2J+1)g_J\mu_B B] \\
&= k_B\left[\frac{\beta\hbar\omega_1/2}{\sinh\left(\beta\hbar\omega_1/2\right)}\right]^2 - k_B\left[\frac{\beta\hbar\omega_2/2}{\sinh\left(\beta\hbar\omega_2/2\right)}\right]^2
\end{aligned}
\tag{29}
$$

where for simplicity we define the frequencies:

$$
\hbar\omega_1 \equiv g_J\mu_B B \qquad \hbar\omega_2 \equiv (2J+1)g_J\mu_B B
\tag{30}
$$

We can define the temperature scale:

$$
\phi \equiv \frac{\hbar\omega}{k_B} = \frac{g_J\mu_B B}{k_B}
\tag{31}
$$

so that the heat capacity becomes:

$$
C_V = k_B\left[\frac{\phi/2}{\sinh\left(\phi/2\right)}\right]^2 - k_B\left[\frac{(2J+1)\phi/2}{\sinh\left[(2J+1)\phi/2\right]}\right]^2
\tag{32}
$$

As shown in the figures, higher $J$ shifts the maximum of the heat capacity towards lower temperatures. In the limit $J \to \infty$, the heat capacity peaks at $T = 0$. Therefore, it is possible to plot the heat capacity as a function of $T$ for a given system and determine $J$ from the position of the peak.

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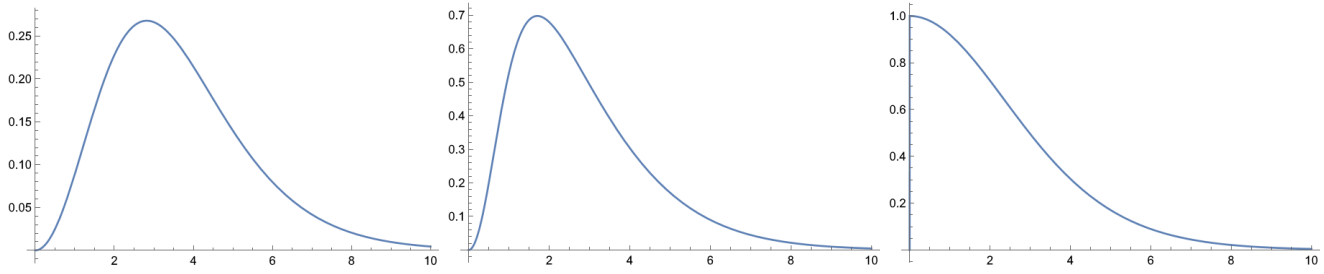
Figure 1: Heat capacity for $J = 1/2$, $J = 3/2$ and $J \to \infty$.

## 2.5

(i)   Consider a single three-dimensional harmonic oscillator with characteristic frequencies $\omega_i$, $i = 1, 2, 3$. The energy levels are given by:

$$E_{n_1,n_2,n_3} = \hbar\omega_1 \left( n_1 + \frac{1}{2} \right) + \hbar\omega_2 \left( n_2 + \frac{1}{2} \right) + \hbar\omega_3 \left( n_3 + \frac{1}{2} \right) \tag{33}$$

The single particle partition function, denoted $Z_1^{(3)}$, is:

$$
\begin{aligned}
Z_1^{(3)} &= \sum_{n_1,n_2,n_3} e^{-\beta E_{n_1,n_2,n_3}} \\
&= \sum_{n_1} e^{-\beta \hbar\omega_1 \left( n_1 + \frac{1}{2} \right)} \sum_{n_2} e^{-\beta \hbar\omega_2 \left( n_2 + \frac{1}{2} \right)} \sum_{n_3} e^{-\beta \hbar\omega_3 \left( n_3 + \frac{1}{2} \right)} \\
&= Z_{1,x} Z_{1,y} Z_{1,z}
\end{aligned}
\tag{34}
$$

Assuming identical frequencies $\omega_i = \omega$, we have:

$$Z_1^{(3)} = Z_1^3 \tag{35}$$

Then the partition function for $N$ non-interacting three-dimensional harmonic oscillators is:

$$Z^{(3)} = (Z_1^{(3)})^N = (Z_1^3)^N = Z_1^{3N} \tag{36}$$

Since the partition function contains all information about the thermodynamics of the system, $N$ non-interacting three-dimensional harmonic oscillators is equivalent to $3N$ one-dimensional harmonic oscillators.

(ii)   Given $\omega = 2\pi\nu = 3.3 \times 10^{13}\,\mathrm{rads}^{-1}$, we have the specific heat:

$$C_V = 3Nk_B \left[ \frac{\beta\hbar\omega/2}{\sinh\left( \beta\hbar\omega/2 \right)} \right]^2 \tag{37}$$

Defining the temperature scale $\theta \equiv \hbar\omega/2k_B = 124.8\,\mathrm{K}$, we have:

$$C_V = 3Nk_B \left[\frac{\theta/T}{\sinh(\theta/T)}\right]^2 \tag{38}$$

The function $x^2/\sinh^2 x$ has a maximum of unity at $x = 0$, so the maximum of $C_V$ is $3Nk_B$ as $T \to \infty$. At room temperature (taken as $T_{\mathrm{room}} = 298\,\mathrm{K}$), we have:

$$\frac{C_V}{3Nk_B} = \left[\frac{\theta/T_{\mathrm{room}}}{\sinh(\theta/T_{\mathrm{room}})}\right]^2 \approx 0.94 \tag{39}$$

This means that the specific heat of the system is already significant at room temperature.

**(iii)** We make the change to temperature scale:

$$\theta = \frac{\hbar\omega}{2k_B} = 748.7\,\mathrm{K} \tag{40}$$

The new fraction for the heat capacity is:

$$\frac{C_V}{3Nk_B} = \left[\frac{\theta/T_{\mathrm{room}}}{\sinh(\theta/T_{\mathrm{room}})}\right]^2 \approx 0.017 \tag{41}$$

which is significantly smaller due to a higher temperature scale.

$\bullet$

## 2.6

**(i)** Suppose that out of the total $N$ particles, $rN$ are the in the higher energy state $E_+$ and $(1-r)N$ are in the lower energy state $E_-$. We assume $r > 0.5$. We could write the entropy as:

$$S = -k_B \sum_{-,+} p_i \ln p_i = -k_B \left[r \ln r + (1 - r) \ln(1 - r)\right] \tag{42}$$

and the internal energy:

$$U = rNE_+ + (1 - r)NE_- \tag{43}$$

But the temperature is defined via the entropy as:

$$T = -\left(\frac{\partial U}{\partial S}\right)_V$$
$$= -\left(\frac{\partial U}{\partial r}\right)_V \left(\frac{\partial r}{\partial S}\right)_V \tag{44}$$
$$= \frac{E_+ - E_-}{k_B[\ln r - \ln(1-r)]}$$

Since $r > 1 - r$ and both quantities are less than unity, we have $\ln r - \ln(1-r) < 0$. Therefore, the effective temperature is negative, which shows that the system cannot be in equilibrium.

**(ii)** The swapping operation is equivalent to the exchange of the ratios $r$ and $1 - r$, i.e., the substitution $r \to 1 - r$. The entropy is invariant under this operation, but the temperature changes sign:

$$T \to \frac{E_+ - E_-}{k_B[\ln(1-r) - \ln r]} \tag{45}$$

**(iii)** Taking instead the limit $r \to 1$, we have $\ln r \to 0$ and $\ln(1-r) \to -\infty$, so that the temperature tends to zero:

$$T \to -\frac{E_+ - E_-}{k_B \ln(1-r)} \to 0 \tag{46}$$

$\bullet$