1

$$g(N,U,V) = f(N)\, V^N\, U^{3N/2}$$

From g we can find the entropy

$$S = k_B \ln g = k_B \ln\left(f(N)\, V^N\, U^{3N/2}\right)$$

$$= k_B \ln\left(f(N)\, V^N\right) + k_B \ln U^{3N/2}$$

$$= k_B \ln\left(f(N)\, V^N\right) + \underbrace{\frac{3Nk_B}{2} \ln U}_{\text{function of } U}$$

From S can find the temperature

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_{N,V} = \left(\frac{\partial\left(\frac{3Nk_B}{2}\ln U\right)}{\partial U}\right)_{N,V}$$

$$= \frac{3Nk_B}{2U} \implies \boxed{U = \frac{3}{2} N k_B T}$$

2. Paramegnetism

a) We know the multiplicity of a chain of N spins, is:

$$g(N, N_\uparrow, N_\downarrow) = \frac{N!}{N_\uparrow!\, N_\downarrow!}$$

$$\underbrace{\uparrow\ \uparrow\ \downarrow\ \downarrow\ \downarrow\ \uparrow\ \downarrow\ \uparrow\ \cdots\cdots}_{N \text{ spins.}}$$

Hence the entropy is given by the formula:

$$S = k_B \ln\left(g(N, N_\uparrow, N_\downarrow)\right)$$

$$= k_B \ln\left(\frac{N!}{N_\uparrow! N_\downarrow!}\right)$$

$$= k_B \ln(N!) - k_B \ln(N_\uparrow!) - k_B \ln(N_\downarrow!)$$

As $N, N_\uparrow, N_\downarrow \gg 1$ individually we may use:

$$\ln(N!) = N\ln(N) - N \quad \text{(Stirling Approx.)}$$

Thus,

$$S = k_B\left(N\ln(N) - N\right) - k_B\left(N_\uparrow \ln(N_\uparrow) - N_\uparrow\right) - k_B\left(N_\downarrow \ln(N_\downarrow) - N_\downarrow\right)$$

~~Defining the~~

Defining the spin excess, $2s = N_\uparrow - N_\downarrow$, we can rewrite the entropy as:

$$(*) \quad S(N,s) = k_B\left(N\ln(N) - N\right)$$
$$- k_B\left(\left(\tfrac{1}{2}N + s\right)\ln\left(\tfrac{1}{2}N+s\right) \cancel{\tfrac{1}{2}(N+s)} - \left(\tfrac{1}{2}N+s\right)\right)$$
$$- k_B\left(\left(\tfrac{1}{2}N - s\right)\ln\left(\tfrac{1}{2}N-s\right) - \left(\tfrac{1}{2}N-s\right)\right)$$
$$= k_B\left[N\ln(N) - \left(\tfrac{1}{2}N+s\right)\ln\left(\tfrac{1}{2}N+s\right) - \left(\tfrac{1}{2}N-s\right)\ln\left(\tfrac{1}{2}N-s\right)\right]$$
$$- k_B\left(N - \tfrac{1}{2}(N+s) - \left(\tfrac{1}{2}N-s\right)\right)$$
$$\boxed{= k_B\left[N\ln(N) - \left(\tfrac{1}{2}N+s\right)\ln\left(\tfrac{1}{2}N+s\right) - \left(\tfrac{1}{2}N-s\right)\ln\left(\tfrac{1}{2}N-s\right)\right]}.$$

* Note we use $N_\uparrow = \frac{1}{2}N + s$
& $N_\downarrow = \frac{1}{2}N - s$

b) By definition the temperature is:

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_N$$

Now, we have $S = S(N, s)$ and $s = s(U)$.
Hence we may write,

$$\frac{1}{T} = \frac{\partial S}{\partial s}\frac{\partial s}{\partial U} \quad \text{by chain rule.}$$

Firstly, noting the total energy of the chain

$$U = -2smB$$

$$\Rightarrow \quad s = -\frac{U}{2mB}$$

$$\therefore \quad \frac{\partial s}{\partial U} = -\frac{1}{2mB}$$

Then, using our expression from a)

$$\frac{\partial S}{\partial s} = \frac{\partial}{\partial s}\left(-k_B\left(\tfrac{1}{2}N+s\right)\ln\left(\tfrac{1}{2}N+s\right) - k_B\left(\tfrac{1}{2}N-s\right)\ln\left(\tfrac{1}{2}N-s\right)\right)$$

$$= -k_B \ln\left(\tfrac{1}{2}N+s\right) - k_B\frac{\left(\tfrac{1}{2}N+s\right)}{\left(\tfrac{1}{2}N+s\right)}$$

$$+ k_B \ln\left(\tfrac{1}{2}N-s\right) - k_B\frac{\left(\tfrac{1}{2}N-s\right)}{-\left(\tfrac{1}{2}N-s\right)}$$

$$= -k_B \left[\ln\left(\tfrac{1}{2}N+s\right) - \ln\left(\tfrac{1}{2}N-s\right) \right]$$

Thus,

$$\frac{\partial S}{\partial U} = \frac{k_B}{2mB}\left[\ln\left(\tfrac{1}{2}N+s\right) - \ln\left(\tfrac{1}{2}N-s\right) \right] = \frac{k_B}{2mB}\left[\ln\left(\frac{\tfrac{1}{2}N+s}{\tfrac{1}{2}N-s} \right) \right].$$

$$\Rightarrow T = \frac{2mB}{k_B}\left[\ln\left(\frac{\tfrac{1}{2}N+s}{\tfrac{1}{2}N-s} \right) \right]^{-1}$$

$$\boxed{= \frac{2mB}{k_B}\left[\ln\left(\frac{N - U/mB}{N + U/mB} \right) \right]^{-1}}$$

where in the last line we use $s = -\dfrac{U}{2mB}$.

c) Rearranging from above:

$$\frac{2mB}{k_B T} = \ln\left(\frac{N - U/mB}{N + U/mB} \right)$$

$$e^{2mB/k_BT} = \frac{N - U/mB}{N + U/mB}$$

$$\Rightarrow \left(N + U/mB\right) e^{2mB/k_BT} = N - U/mB$$

p.t.o.

$$U = NmB\left[\frac{1 - e^{2mB/k_BT}}{1 + e^{2mB/k_BT}}\right]$$

$$= NmB\left[\frac{e^{-mB/k_BT} - e^{mB/k_BT}}{e^{-mB/k_BT} + e^{mB/k_BT}}\right] \cdot \frac{e^{mB/k_BT}}{e^{mB/k_BT}}$$

$$= NmB \cdot \frac{-\sinh\left(\frac{mB}{k_BT}\right)}{\cosh\left(\frac{mB}{k_BT}\right)}$$ (see definition of $\cosh(x)$, $\sinh(x)$)

$$\boxed{= -NmB \tanh\left(\frac{mB}{k_BT}\right)}$$

d) For large T we have $k_BT \gg mB$

i.e. $\frac{mB}{k_BT} \ll 1$

The taylor expansion for $\tanh(x)$ for $x \ll 1$ is:

$$\tanh(x) \simeq x$$

Hence we may write

$$U \simeq -NmB\left(\frac{mB}{k_BT}\right) \quad \text{for } k_BT \gg mB$$

$$\simeq -N\frac{m^2B^2}{k_BT}$$

Using $\langle U \rangle = -2\langle s \rangle mB$ we can express the fractional magnetization as:

$$-2\langle s \rangle mB \approx -\frac{Nm^2B^2}{k_BT}$$

$$\Rightarrow \frac{2\langle s \rangle}{N} \approx \frac{mB}{k_BT}$$

Thus we indeed get a scaling of $1/T$ for the fractional magnetization, consistent with Curie's law.

e) For $T \to 0$, $\frac{mB}{k_BT} \to \infty$.

For such a case we note,

$$\tanh(x) \to 1 \quad \text{as} \quad x \to \infty$$

Hence we rewrite the energy as:

$$U \approx -NmB.$$

This is consistent as it implies all spins align at low temperature, minimising the energy, i.e.

$$\langle s \rangle = \frac{N}{2}$$

Question 3: Paramagnetism (continjued).

a) see attached plots.

b) By definition the heat capacity is given by:

$$C_B = \left(\frac{\partial \langle U \rangle}{\partial T}\right)_{N,B}$$

Using $\langle U \rangle$ derived in Question 4, this becomes:

$$C_B = -NmB \cdot \frac{\partial}{\partial T}\left(\tanh\left(\frac{mB}{k_B T}\right)\right)$$

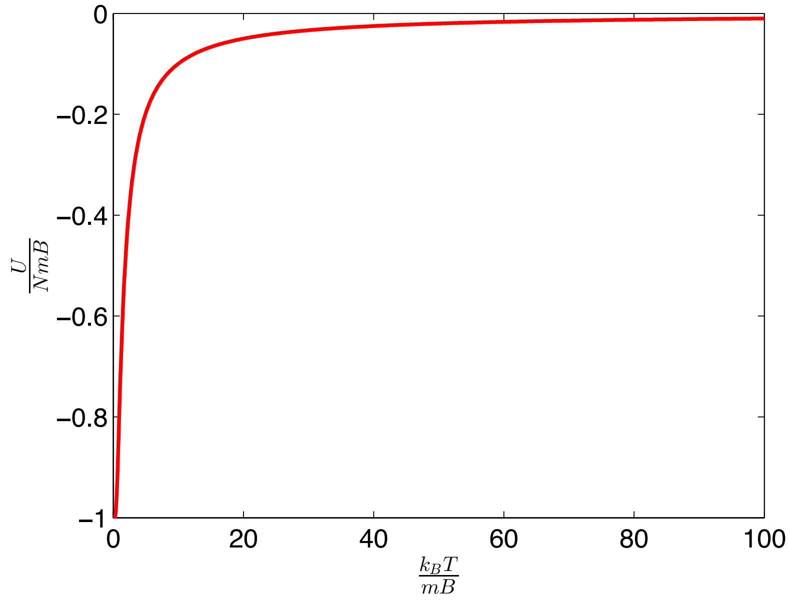
$$= \frac{Nm^2B^2}{k_B T^2} \cdot \frac{1}{\cosh^2\left(\frac{mB}{k_B T}\right)}$$

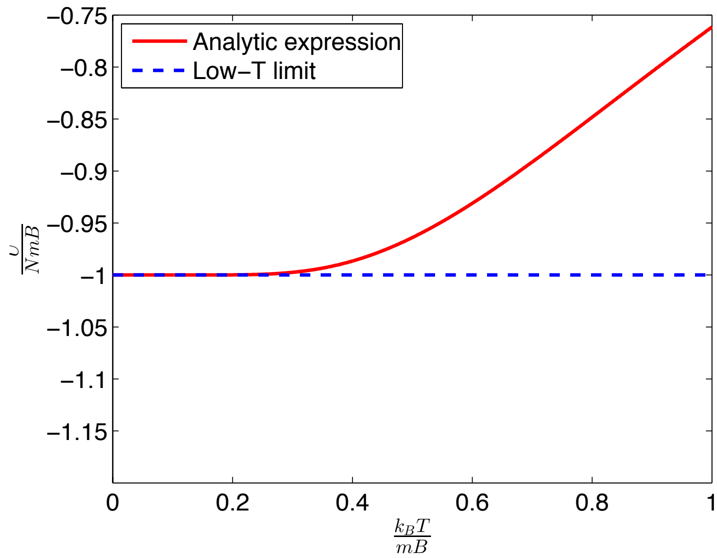
For $T \to 0$, ~~we~~ $k_B T \ll mB$

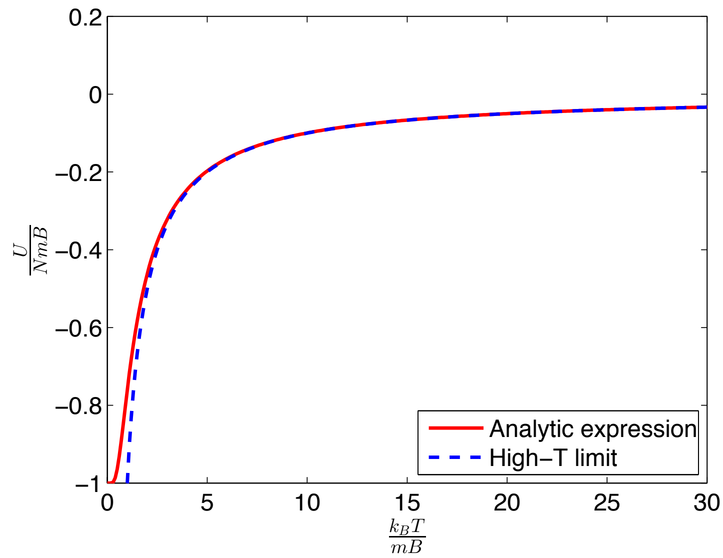
i.e. $\cosh\left(\frac{mB}{k_B T}\right) \simeq \frac{e^{mB/k_B T}}{2}$ [see definition of ~~coth~~ cosh]

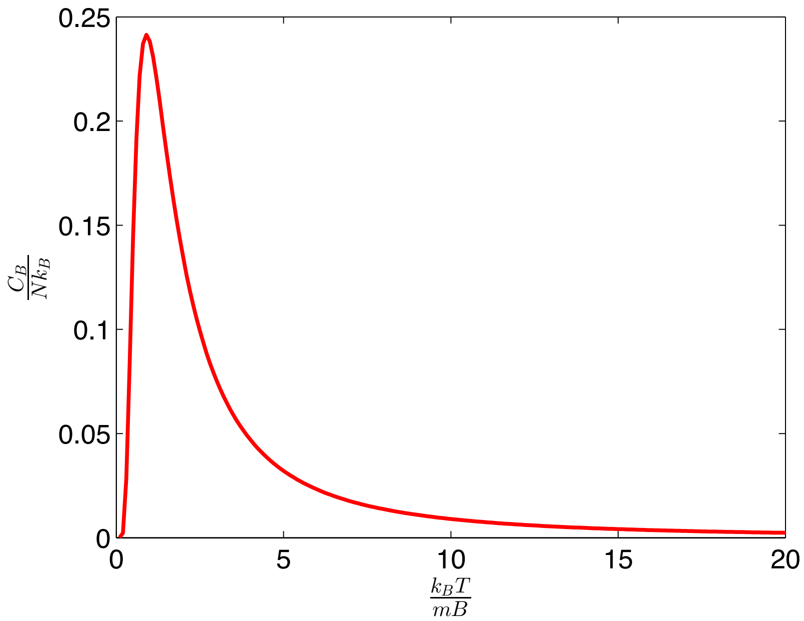
$$\Rightarrow C_B \approx \frac{Nm^2B^2}{k_B T^2} \cdot \frac{4}{e^{2mB/k_B T}}$$

$$\simeq \frac{4Nm^2B^2}{k_B} \cdot \frac{1}{T^2} \cdot e^{-2mB/k_B T}$$


$\frac{U}{NmB}$
$\frac{k_BT}{mB}$


Analytic expression
Low−T limit
$\frac{U}{NmB}$
$\frac{k_BT}{mB}$


Analytic expression
High−T limit
$\frac{U}{NmB}$
$\frac{k_BT}{mB}$


$\frac{C_B}{Nk_B}$
$\frac{k_BT}{mB}$

Thus for $T \to 0$, we expect the heat capacity to exponentially ~~decay~~ decay.

For $T \to \infty$, $k_B T \gg mB$.

ie. $\cosh\left(\frac{mB}{k_B T}\right) \approx 1 + \frac{1}{2}\left(\frac{mB}{k_B T}\right)^2 + \ldots$ (taylor series)

Hence,

$$C_B = \frac{Nm^2B^2}{k_B T^2} \cdot \frac{1}{\left(1+\frac{1}{2}\left(\frac{mB}{k_B T}\right)^2\right)^2}$$

$$\approx \frac{Nm^2B^2}{k_B T^2} \cdot \left[1 - \left(\frac{mB}{k_B T}\right)^2\right] *$$

$$\approx Nk_B \cdot \left(\frac{mB}{k_B T}\right)^4 \quad \text{for } T \to \infty$$

* Note here we use: $(1+ax)^n \approx 1 + nax$ for $ax \ll 1$

Hence for $T \to \infty$ we expect the heat capacity to go to zero as $1/T^4$.

c)

We assume the multiplicity of the chain can be approximated as:

$$g(N,s) = g(N,0)\, e^{-2s^2/N}$$

which is valid for: $\underline{|s| \ll N}$ & $\underline{N \gg 1}$.

Then the entropy is given by:

$$S = k_B \log(g)$$

$$= k_B \log(g(N,0)) - \frac{2k_B s^2}{N}$$

Trivially we then calculate the equilibrium temperature as:

$$\frac{1}{T} = \left(\frac{\partial S}{\partial U}\right)_N = \frac{\partial S}{\partial s}\frac{\partial s}{\partial U}$$

Noting $U = -2smB$ from Q4,

$$\Rightarrow \frac{\partial s}{\partial U} = \frac{\partial}{\partial U}\left(\frac{U}{-2mB}\right) = \frac{-1}{2mB}$$

$$\Rightarrow \frac{1}{T} = -\frac{4k_B s}{N} \cdot \frac{-1}{2mB}$$

$$= \frac{2k_B s}{NmB}$$

Rewriting s in terms of U,

$$T = -\frac{N m^2 B^2}{k_B U}$$

which can be inverted to give the thermal average energy:

$$U = -\frac{N m^2 B^2}{k_B T}$$

which agrees with the high temperature limit derived in Q4.

Note that our method does not recover the low-temperature behaviour as the initial approximations are invalid. Namely as $T \to 0$ we intuitively expect all spins to align, which would imply $|s| \sim N$, explicitly contradicting the approximation $|s| \ll N$.

Question 4: The Einstein Model of a Solid

a) We treat each atom in the lattice as 3 harmonic oscillators (one each to correspond to motion in the x, y, z directions).

Each oscillator has the same frequency, ω, and for $\frac{N}{3}$ atoms, there exist N oscillators.

If we assume a total of q_{tot} quanta to be shared then,

$$U = q_{tot} \hbar\omega = N\hbar\omega$$

Using the sticks and ~~boxes~~ balls method, (see lecture notes) it can easily be shown

$$g(N,q) = \frac{(q+N-1)!}{q!(N-1)!}$$

is the multiplicity where $q = q_{tot}$.

Following the derivation of QS in problem set 1 we may calculate the entropy, equilibrium temperature etc. We refer the student to the solutions of that problem set for the full results. In the following we only require the result:

$$U = \frac{N\hbar\omega}{e^{\hbar\omega/k_BT} - 1}$$

which is the thermal equilibrium total energy for a given temperature T.

b) We use the expression for U found in a) and consider the limits of high & low temperature.

For $T \to \infty$, $k_B T \gg \hbar\omega$, we may expand

$$e^{\hbar\omega/k_B T} \simeq 1 + \frac{\hbar\omega}{k_B T} + \dots \quad \text{(taylor series)}$$

We then ~~rewrite~~ rewrite the total energy as:

$$U \simeq \frac{N\hbar\omega}{1 + \frac{\hbar\omega}{k_B T} - 1} \simeq N\hbar\omega . \frac{k_B T}{\hbar\omega}$$

$$\simeq N k_B T. \quad (\propto T)$$

This result is consistent with the equi-partition theorem for classical particles. Each oscillator has energy $k_B T$ as the Hamiltonian is quadratic in both position & momentum. ~~Thus for $\frac{N}{3}$ atoms, with~~

For $T \to 0$, $k_B T \ll \hbar\omega$, we note that

$$e^{\hbar\omega/k_B T} \gg 1$$

Hence we write the total energy as:

$$\cancel{U = N\hbar\omega} \quad U = N\hbar\omega\, e^{-\hbar\omega/k_B T}$$

ie. the energy decays exponentially as $T \to 0$

$\Rightarrow$ See attached plots for U vs. T.

c) Using the expression for U, the heat capacity is:

$$C_V = \left(\frac{\partial U}{\partial T}\right)_{N,V}$$

$$= \frac{\partial}{\partial T}\left[\frac{N\hbar\omega}{e^{\hbar\omega/k_B T} - 1}\right]$$

$$= \cancel{\frac{N(\hbar\omega)^2}{k_B T^2}} \; N k_B \cdot \left(\frac{\hbar\omega}{k_B T}\right)^2 \cdot \frac{e^{\hbar\omega/k_B T}}{\left(e^{\hbar\omega/k_B T} - 1\right)^2}$$

d) For $T \to \infty$, $k_B T \gg \hbar\omega$ and we again use:

$$e^{\hbar\omega/k_BT} \simeq 1 + \frac{\hbar\omega}{k_BT}$$

Hence,

$$C_V \simeq Nk_B\left(\frac{\hbar\omega}{k_BT}\right)^2 \cdot \frac{1+\hbar\omega/k_BT}{\left(\frac{\hbar\omega}{k_BT}\right)^2}$$

$$\simeq Nk_B\left(1+\hbar\omega/k_BT\right)$$

$$\simeq Nk_B \quad \text{for} \quad \frac{\hbar\omega}{k_BT} \ll 1$$

Again, this is the expected result for a classical system due to the ~~equi-p~~ equipartition theorem.

For $T \to 0$, $k_BT \ll \hbar\omega$, we use:

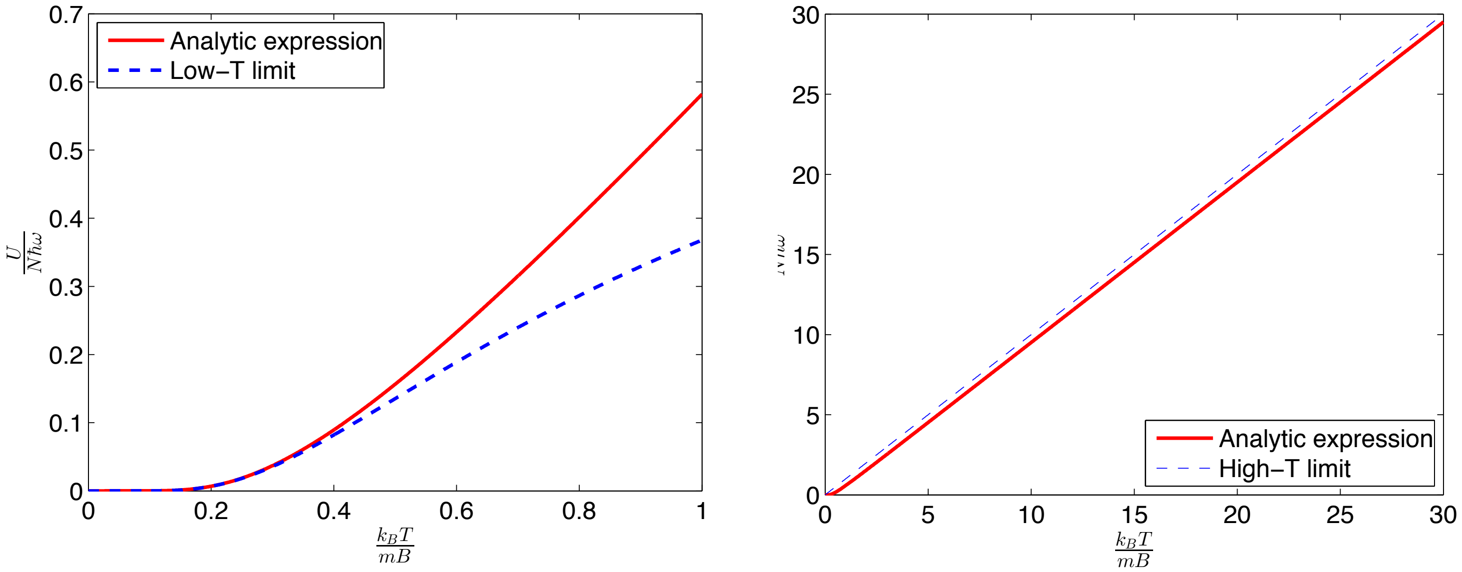
$$e^{\hbar\omega/k_BT} \gg 1$$

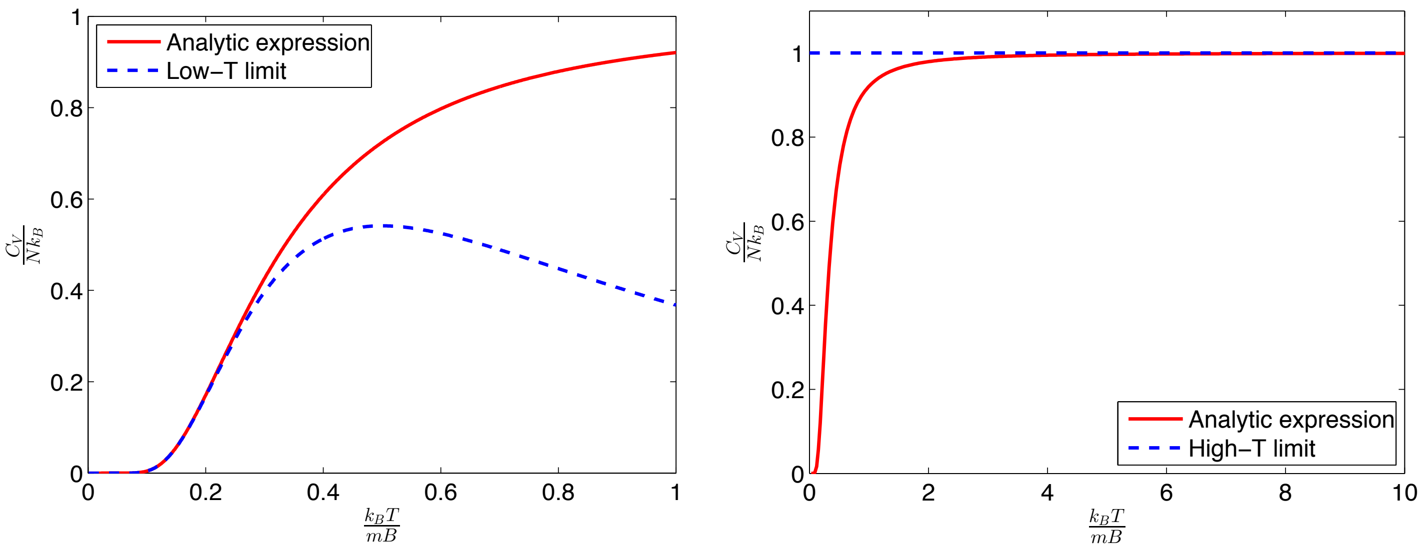
Hence,

$$C_V \simeq Nk_B\left(\frac{\hbar\omega}{k_BT}\right)^2 \frac{e^{\hbar\omega/k_BT}}{e^{2\hbar\omega/k_BT}}$$

$$\simeq Nk_B\left(\frac{\hbar\omega}{k_BT}\right)^2 e^{-\hbar\omega/k_BT}$$

$\Rightarrow$ We expect an exponential decay in the heat capacity for low T.


Analytic expression
Low−T limit
Analytic expression
High−T limit


Analytic expression
Low−T limit
Analytic expression
High−T limit