The phonon heat capacity for 1D, 2D and 3D system

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(Date: September 29, 2018)

When I taught the Phys.411-511 (Statistical Thermodynamics, 2016) using the textbook of Huang, Introduction to Statistical Mechanics, I realized that the definition of the density of states for the statistical mechanics is different from that for the solid state physics even if we solve the same problem. In solid state physics, the velocity of the transverse mode is in general different from that of the longitudinal mode, while these velocities are the same in the statistical mechanics. In the 2D phonon, we use the approximation

$$\frac{2}{\overline{v}^2} = \frac{1}{v_T{}^2} + \frac{1}{v_L{}^2} \qquad \text{for the solid state physics}$$

and

$$v = v_T = v_L \qquad \text{for the statistical mechanics.}$$

1. 2D phonon

Show that the Debye model of a 2-dimensional crystal predicts that the low temperature heat capacity is proportional to T^2. Solve the problem by answering the following questions.

(a) Find the expression of the density of states.
(b) Find the expression (without any approximation) for the internal energy.
(c) Find the expression of the heat capacity with integral (you do not have to calculate the integral).
(d) Find the expression of the entropy.

((Solution-1))

(a) Density of states

There is one allowed states per $(2\pi/L)^2$ in 2D $\boldsymbol{k}$-space. In other words, there are

$$\frac{1}{(2\pi)^2/L^2},$$

states per unit area of 2D $\boldsymbol{k}$ space, for each polarization and for each branch

The density of states is defined by

$$D(\omega)d\omega = \frac{dk_x dk_y}{(2\pi)^2 / L^2} = \frac{2\pi k dk}{(2\pi)^2 / L^2} = \frac{L^2 k dk}{2\pi},$$

using the linear dispersion relation, $\omega = vk$,

$$D(\omega) = \frac{L^2 \omega}{2\pi v^2},$$

which is proportional to ω.

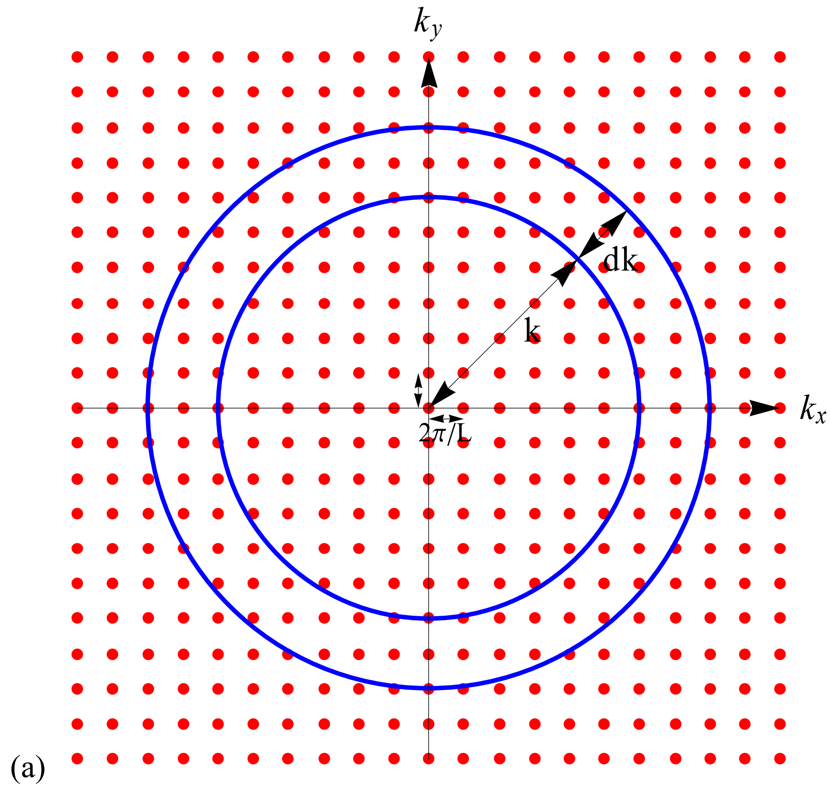

Fig. Density of states for the 2D ***k***-space. There is one state per area $\left(\frac{2\pi}{L}\right)^2$ of the reciprocal lattice plane.

(b) Internal energy

We calculate the heat capacity of 2D systems in the Debye approximation. The thermal energy is given by

$$U = \int d\omega D(\omega)\hbar\omega < n(\omega) > = \int_0^{\omega_D} d\omega \left(\frac{L^2}{2\pi}\right)\frac{\omega}{v^2}\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}\right),$$

for each polarization type (1 TA, 1 LA) The phonon velocity for the longitudinal mode and the transverse mode is given by v_L and v_T, respectively. Then the total energy is

$$U = \left(\frac{L^2}{2\pi}\right)\left(\frac{1}{{v_L}^2}+\frac{1}{{v_T}^2}\right)\int_0^{\omega_D} d\omega\hbar\omega^2\left(\frac{1}{e^{\beta\hbar\omega}-1}\right)$$

We assume that

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$$\frac{2}{v^2} = \frac{1}{{v_L}^2}+\frac{1}{{v_T}^2}$$

and $v_L = v_T$, leading to $v = v_L = v_T$. Then we get

$$U = 2\left(\frac{\hbar L^2}{2\pi v^2}\right)\int_0^{\omega_D} d\omega\left(\frac{\omega^2}{e^{\beta\hbar\omega}-1}\right)$$
$$= 2\left(\frac{\hbar L^2}{2\pi v^2}\right)\frac{{k_B}^3T^3}{\hbar^3}\int_0^{\Theta/T} dx\left(\frac{x^2}{e^x-1}\right)$$

where $x = \beta\hbar\omega$, $k_B\Theta = \hbar\omega_D$

We note that

$$N = \int_0^{\omega_D} d\omega D(\omega) = \int_0^{\omega_D} d\omega\frac{L^2}{2\pi}\frac{\omega}{v^2} = \frac{L^2{\omega_D}^2}{4\pi v^2},$$

or

$${\omega_D}^2 = 4\pi v^2\frac{N}{L^2} = \frac{{k_B}^2}{\hbar^2}\Theta^2,$$

Thus we have

$$\frac{U}{N} = 4k_B T \left(\frac{T}{\Theta}\right)^2 \int_0^{\Theta/T} dx \frac{x^2}{e^x - 1}$$

In the low temperature limit, we have

$$\int_0^\infty dx \frac{x^2}{e^x - 1} = 2\varsigma(3) = 2.40411, \qquad \varsigma(3) = 1.20205$$

$$U = 4Nk_B T \left(\frac{T}{\Theta}\right)^2 \varsigma(3)$$

In the high temperature limit

$$\frac{U}{N} \approx 4k_B T \left(\frac{T}{\Theta}\right)^2 \int_0^{\Theta/T} dx x = 2k_B T ,$$

since

$$\frac{x^2}{e^x - 1} \approx x .$$

(c) The heat capacity

The heat capacity is

$$C = \frac{\partial U}{\partial T} = 24\varsigma(3) Nk_B \left(\frac{T}{\Theta}\right)^2 = 28.8492 Nk_B \left(\frac{T}{\Theta}\right)^2 .$$

The entropy is calculated as

$$S = \int \frac{C}{T} dT$$
$$= 24\varsigma(3) N k_B \int_0^T \frac{T}{\Theta^2} dT$$
$$= 12\varsigma(3) N k_B \left(\frac{T}{\Theta}\right)^2$$
$$= 14.4246 N k_B \left(\frac{T}{\Theta}\right)^2$$

((**Solution-2**))

This method is correct only if the phonon velocity is independent of the polarization ($v_t = v_l = v$).

The density of states is defined by

$$D_2(\omega) d\omega = 2\frac{dk_x dk_y}{(2\pi)^2 / L^2} = 2\frac{2\pi k dk}{(2\pi)^2 / L^2} = 2\frac{L^2 k dk}{2\pi},$$

using the linear dispersion relation, $\omega = vk$,

$$D_2(\omega) = \frac{L^2 \omega}{\pi v^2},$$

which is proportional to ω. Note that the factor 2 of the density of states comes from two types of polarization (1 TA and 1 LA). Then we have

$$2N = \int_0^\infty D_2(\omega) d\omega = \int_0^{\omega_D} \frac{L^2 \omega}{\pi v^2} d\omega = \frac{L^2 {\omega_D}^2}{2\pi v^2}$$

or

$${\omega_D}^2 = 4\pi v^2 \frac{N}{L^2} = \frac{{k_B}^2}{\hbar^2} \Theta^2$$

or

$$N = \frac{{k_B}^2 \Theta^2}{4\pi v^2 \hbar^2} L^2$$

The total energy is

$$U = \int d\omega D_2(\omega)\hbar\omega < n(\omega) > = \int_0^{\omega_D} d\left(\frac{L^2\omega}{\pi v^2}\right)\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}\right)$$

or

$$\begin{aligned} U &= \left(\frac{\hbar L^2}{\pi v^2}\right)\int_0^{\omega_D} d\omega\left(\frac{\omega^2}{e^{\beta\hbar\omega}-1}\right) \\ &= \left(\frac{\hbar L^2}{\pi v^2}\right)\frac{k_B{}^3T^3}{\hbar^3}\int_0^{\Theta/T} dx\left(\frac{x^2}{e^x-1}\right) \end{aligned}$$

The ratio U/N can be evaluated as

$$\begin{aligned} \frac{U}{N} &= \frac{4\pi v^2\hbar^2}{k_B{}^2\Theta^2L^2}\left(\frac{\hbar L^2}{\pi v^2}\right)\frac{k_B{}^3T^3}{\hbar^3}\int_0^{\Theta/T} dx\left(\frac{x^2}{e^x-1}\right) \\ &= 4k_BT\left(\frac{T}{\Theta}\right)^2\int_0^{\Theta/T} dx\left(\frac{x^2}{e^x-1}\right) \end{aligned}$$

In the low temperature limit, we have

$$\int_0^{\infty} dx\frac{x^2}{e^x-1} = 2\varsigma(3) = 2.40411, \qquad \varsigma(3) = 1.20205$$

$$U = 4Nk_BT\left(\frac{T}{\Theta}\right)^2\varsigma(3)\,.$$

In the high temperature limit

$$\frac{U}{N} \approx 4k_BT\left(\frac{T}{\Theta}\right)^2\int_0^{\Theta/T} dxx = 2k_BT$$

The heat capacity is

$$C = \frac{\partial U}{\partial T} = 24\varsigma(3)Nk_B\left(\frac{T}{\Theta}\right)^2 = 28.8492Nk_B\left(\frac{T}{\Theta}\right)^2$$

The entropy is calculated as

$$S = \int \frac{C}{T} dT$$
$$= 24\varsigma(3) N k_B \int_0^T \frac{T}{\Theta^2} dT$$
$$= 12\varsigma(3) N k_B \left(\frac{T}{\Theta}\right)^2$$
$$= 14.4246 N k_B \left(\frac{T}{\Theta}\right)^2$$

2. Exact expression of the heat capacity for the 2D system

We start with the internal energy given by

$$U = \left(\frac{\hbar L^2}{\pi v^2}\right) \int_0^{\omega_D} d\omega \left(\frac{\omega^2}{e^{\beta\hbar\omega} - 1}\right)$$

The heat capacity is

$$C = \frac{dU}{dT} = \frac{d\beta}{dT}\frac{\partial U}{\partial \beta} = \frac{1}{k_B T^2} \frac{\hbar^2 L^2}{\pi v^2} \int_0^{\omega_D} d\omega \frac{\omega^3 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

or

$$C = \frac{1}{k_B T^2} \frac{\hbar^2 L^2}{\pi v^2} \left(\frac{k_B T}{\hbar}\right)^4 \int_0^{\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$
$$= \frac{L^2}{\pi \hbar^2 v^2} k_B{}^3 T^2 \int_0^{\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$

Then the ratio

$$\frac{C}{N} = \frac{4\pi v^2 \hbar^2}{k_B{}^2 \Theta^2 L^2} \frac{L^2}{\pi \hbar^2 v^2} k_B{}^3 T^2 \int_0^{\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$
$$= 4 k_B \left(\frac{T}{\Theta}\right)^2 \int_0^{\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$

or

$$C = 4Nk_B\left(\frac{T}{\Theta}\right)^2 \int_0^{2\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$

When $N = N_A$,

$$\frac{C}{R} = 4\left(\frac{T}{\Theta}\right)^2 \int_0^{2\Theta/T} dx \frac{x^3 e^x}{(e^x - 1)^2}$$

This is a universal function of only a ratio T/Θ. We make a plot of this function by using the Mathematica.

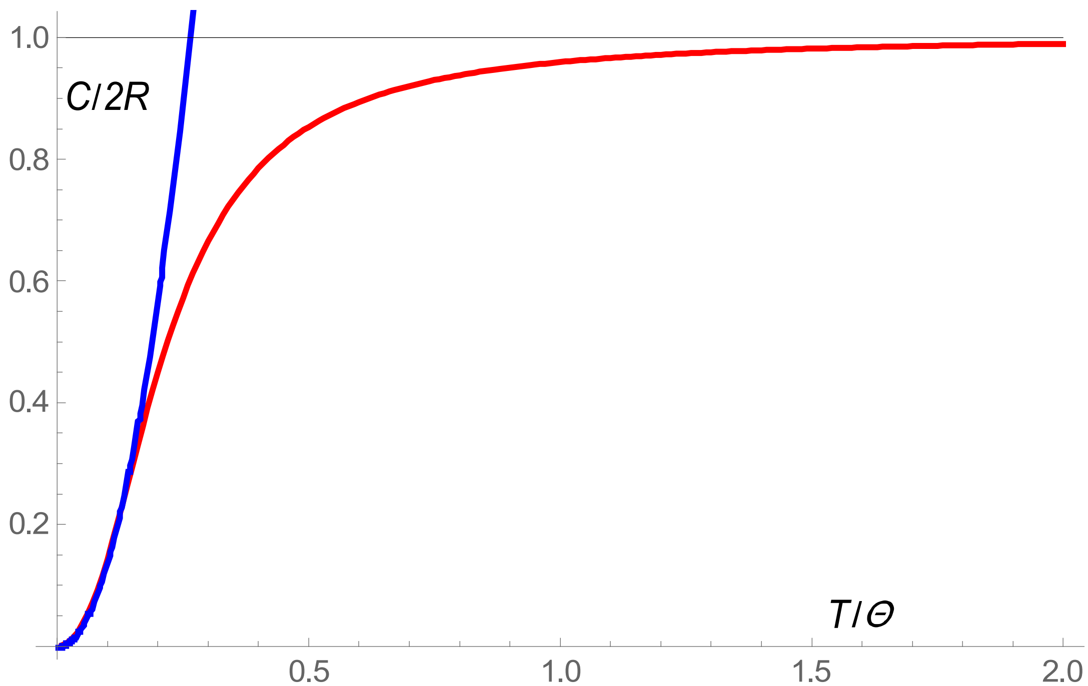

Fig. Plot of $C/(2R)$ as a function of T/Θ for the 2D phonon system. The red line denotes the exact expression, while the blue line denotes the low temperature limit. $C/(2R)$ tends to the unity in the high temperature limit.

3. 3D phonon

Show that the Debye model of a 3-dimensional crystal predicts that the low temperature heat capacity is proportional to T^3. Solve the problem by answering the following questions.

(a) Find the expression of the density of states.

(b) Find the expression (without any approximation) for the internal energy.

(c) Find the expression of the heat capacity with integral (you do not have to calculate the integral).

(d) Find the expression of the entropy.

((Solution-1))

(a) Density of states

There is one allowed states per $(2\pi/L)^3$ in 3D ***k***-space. In other words, there are

$$\frac{1}{(2\pi)^3/L^3},$$

states per unit area of 3D ***k*** space, for each polarization and for each branch

The density of states is defined by

$$D(\omega)d\omega = \frac{dk_x dk_y dk_z}{(2\pi)^3/L^3} = \frac{4\pi k^2 dk}{(2\pi)^3/L^3} = \frac{L^3 k^2 dk}{2\pi^2},$$

using the linear dispersion relation, $\omega = vk$,

$$D(\omega) = \frac{L^3\omega^2}{2\pi^2 v^3},$$

(b) Internal energy

We calculate the heat capacity of 2D systems in the Debye approximation. The thermal energy is given by

$$\begin{aligned} U &= \int d\omega D(\omega)\hbar\omega < n(\omega) > \\ &= \int_0^{\omega_D} d\omega \frac{L^3\omega^2}{2\pi^2 v^3}\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}\right), \\ &= \frac{\hbar L^3}{2\pi^2}\frac{1}{v^3}\int_0^{\omega_D} d\omega\omega^3\left(\frac{1}{e^{\beta\hbar\omega}-1}\right) \end{aligned}$$

for each polarization type (2 TA, 1 LA) The phonon velocity for the longitudinal mode and the transverse mode is given by v_L and v_T, respectively. Then the total energy combining three branches is

$$U = \left(\frac{\hbar L^3}{2\pi^2}\right)\left(\frac{1}{v_L{}^3} + \frac{2}{v_T{}^3}\right)\int_0^{\omega_D} d\omega\omega^3 \left(\frac{1}{e^{\beta\hbar\omega} - 1}\right)$$

We assume that

.

$$\frac{3}{v^3} \to \frac{1}{v_L{}^3} + \frac{2}{v_T{}^3} = \frac{3}{v^3}$$

If $v_L = v_T$, we have $v = v_L = v_T$. Under this condition, we get

$$U = 3\left(\frac{\hbar L^3}{2\pi^2 v^3}\right)\int_0^{\omega_D} d\omega \left(\frac{\omega^3}{e^{\beta\hbar\omega} - 1}\right)$$
$$= 3\left(\frac{\hbar L^3}{2\pi^2 v^3}\right)\frac{k_B{}^4 T^4}{\hbar^4}\int_0^{\Theta/T} dx \left(\frac{x^3}{e^x - 1}\right)$$

where $x = \beta\hbar\omega$, $k_B\Theta = \hbar\omega_D$

We note that

$$N = \int_0^{\omega_D} d\omega D(\omega) = \int_0^{\omega_D} d\omega \frac{L^3\omega^2}{2\pi^2 v^3} = \frac{L^3\omega_D{}^3}{6\pi^2 v^3},$$ for each branch,

or

$$\omega_D{}^3 = 6\pi^2 v^3 \frac{N}{L^3} = \frac{k_B{}^3}{\hbar^3}\Theta^3, \qquad \Theta = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N}{V}\right)^{1/3}$$

or

$$\Theta = \frac{\hbar v}{k_B}\left(\frac{6\pi^2 N}{V}\right)^{1/3} = \frac{\hbar v}{k_B}\left(6\pi^2 n\right)^{1/3}$$ (Debye temperature)

with the number density, $n = \frac{N}{V}$. Then we have

$$\frac{U}{N} = 9k_B T\left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} dx \frac{x^3}{e^x - 1}$$

In the low temperature limit, we have

$$\int_0^{\infty} dx \frac{x^3}{e^x - 1} = \frac{\pi^4}{15} = 6.49394,$$

and

$$U = \frac{3\pi^4}{5} Nk_B T\left(\frac{T}{\Theta}\right)^3$$

In the high temperature limit

$$U = 3Nk_B T$$

since

$$\frac{x^3}{e^x - 1} \approx x^2 .$$

(c) The heat capacity

The heat capacity is

$$C = \frac{\partial U}{\partial T} = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\Theta}\right)^3 = 233.782 Nk_B \left(\frac{T}{\Theta}\right)^3$$

Which is the Debye T^3 approximation. The entropy is calculated as

$$S = \int \frac{C}{T} dT$$

$$= \frac{12\pi^4}{5} Nk_B \int_0^T \frac{T^2}{\Theta^3} dT$$

$$= \frac{4\pi^4}{5} Nk_B \left(\frac{T}{\Theta}\right)^3$$

((Solution-2))

This method is correct only if the phonon velocity is independent of the polarization ($v_t = v_l = v$). The density of states is defined by

$$D_3(\omega)d\omega = 3\frac{dk_x dk_y dk_z}{(2\pi)^2 / L^2} = 3\frac{4\pi k^2 dk}{(2\pi)^3 / L^3} = 3\frac{L^3 k^2 dk}{2\pi^2},$$

using the linear dispersion relation, $\omega = vk$,

$$D_3(\omega) = \frac{3L^3\omega^2}{2\pi^2 v^3},$$

which is proportional to ω^2. Note that the factor 3 of the density of states comes from three types of polarization (2 TA and 1 LA). Then we have

$$3N = \int_0^\infty D_3(\omega)d\omega = \int_0^{\omega_D} \frac{3L^3\omega^2}{2\pi^2 v^3} d\omega = \frac{L^3 {\omega_D}^3}{2\pi^2 v^3}$$

or

$${\omega_D}^3 = 6\pi^2 v^3 \frac{N}{L^3} = \frac{{k_B}^3 \Theta^3}{\hbar^3}$$

or

$$N = \frac{{k_B}^3 \Theta^3}{6\pi^2 v^3 \hbar^3} L^3$$

The total energy is

$$U = \int d\omega D_3(\omega)\hbar\omega < n(\omega) > = \int_0^{\omega_D} d\omega \frac{3L^3\omega^2}{2\pi^2 v^3}\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}\right)$$

or

$$U = \frac{3\hbar L^3}{2\pi^2 v^3}\int_0^{\omega_D} d\omega\left(\frac{\omega^3}{e^{\beta\hbar\omega}-1}\right)$$
$$= \frac{3\hbar L^3}{2\pi^2 v^3}\frac{k_B{}^4 T^4}{\hbar^4}\int_0^{\Theta/T} dx\left(\frac{x^2}{e^x-1}\right)$$

The ratio U/N can be evaluated as

$$\frac{U}{N} = \frac{6\pi^2 v^3\hbar^3}{k_B{}^3\Theta^3 L^3}\frac{3\hbar L^3}{2\pi^2 v^3}\frac{k_B{}^4 T^4}{\hbar^4}\int_0^{\Theta/T} dx\left(\frac{x^3}{e^x-1}\right)$$
$$= 9k_B T\left(\frac{T}{\Theta}\right)^3\int_0^{\Theta/T} dx\left(\frac{x^3}{e^x-1}\right)$$

In the low temperature limit, we have

$$\int_0^{\infty} dx\frac{x^3}{e^x-1} = \frac{\pi^4}{15}$$

$$U = \frac{9\pi^4}{15}Nk_B T\left(\frac{T}{\Theta}\right)^3.$$

In the high temperature limit

$$U \approx 9Nk_B T\left(\frac{T}{\Theta}\right)^3\int_0^{\Theta/T} dx x^2 = 3Nk_B T$$

The heat capacity is

$$C = \frac{\partial U}{\partial T} = \frac{12\pi^4}{5}Nk_B\left(\frac{T}{\Theta}\right)^3 = 233.782Nk_B\left(\frac{T}{\Theta}\right)^3.$$

The entropy is calculated as

$$S = \int \frac{C}{T} dT$$
$$= \frac{12}{5}\pi^4 N k_B \int_0^T \frac{T^2}{\Theta^3} dT$$
$$= \frac{4}{5}\pi^4 N k_B \left(\frac{T}{\Theta}\right)^3$$

4. Exact expression of heat capacity for the 3D system

We start with the internal energy given by

$$U = \frac{3\hbar L^3}{2\pi^2 v^3} \int_0^{\omega_D} d\omega \left(\frac{\omega^3}{e^{\beta\hbar\omega} - 1} \right)$$

The heat capacity C is calculated as

$$C = \frac{\partial U}{\partial T}$$
$$= \frac{d\beta}{dT} \frac{\partial U}{\partial \beta}$$
$$= -\frac{1}{k_B T^2} \frac{3\hbar L^3}{2\pi^2 v^3} \int_0^{\omega_D} d\omega \frac{\partial}{\partial \beta} \left(\frac{\omega^3}{e^{\beta\hbar\omega} - 1} \right)$$
$$= \frac{3\hbar^2 L^3}{2\pi^2 v^3 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$

or

$$\frac{C}{N} = \frac{6\pi^2 v^3 \hbar^3}{k_B{}^3 \Theta^3 L^3} \frac{3\hbar^2 L^3}{2\pi^2 v^3 k_B T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$
$$= \frac{9}{k_B{}^4 \Theta^3} \frac{\hbar^5}{T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$
$$= 9 k_B \left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} dx \frac{x^4 e^x}{\left(e^x - 1\right)^2}$$

or

$$C = 9Nk_B\left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

We assume that $N = N_A$. Since $R = N_A k_B$ (gas constant),

$$\frac{C}{3R} = 3\left(\frac{T}{\Theta}\right)^3 \int_0^{\Theta/T} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

This is a universal function of only a ratio T/Θ. We make a plot of this function by using the Mathematica.

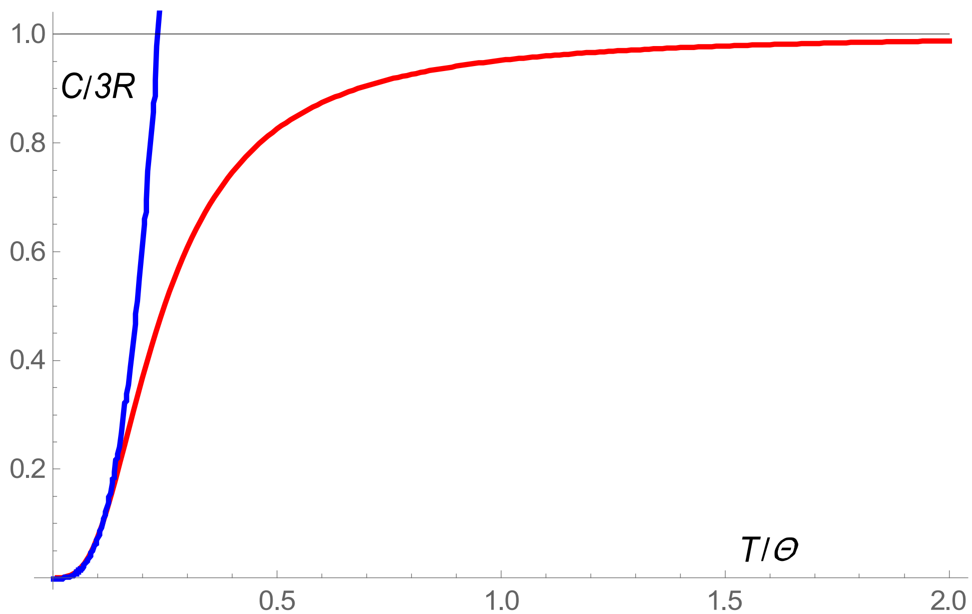

Fig. Plot of $C/(3R)$ as a function of T/Θ for the 3D phonon system. The red line denotes the exact expression, while the blue line denotes the low temperature limit. $C/(3R)$ tends to the unity in the high temperature limit.

5. 1D phonon

Show that the Debye model of a 1-dimensional (1D) crystal predicts that the low temperature heat capacity is proportional to T. Solve the problem by answering the following questions.

(a) Find the expression of the density of states.

(b) Find the expression (without any approximation) for the internal energy.

(c) Find the expression of the heat capacity with integral (you do not have to calculate the integral).

(d) Find the expression of the entropy.

((Solution-1))

(a) Density of states

There is one allowed state per $(2\pi/L)$ in 1D ***k***-space. In other words, there are

$$\frac{1}{2\pi / L},$$

states per unit length of 1D k space.

The density of states is defined by

$$D(\omega)d\omega = 2\frac{dk_x}{2\pi / L} = \frac{L}{\pi}dk_x = \frac{L}{\pi v}d\omega,$$

using the linear dispersion relation, $\omega = vk$,

$$D(\omega) = \frac{L}{\pi v},$$

which is independent of ω . Note that the factor 2 comes from the property that $\omega(-k) = \omega(k)$

Internal energy

We calculate the heat capacity of 1D systems in the Debye approximation. The thermal energy is given by

$$U = \int d\omega D(\omega)\hbar\omega < n(\omega) > = \frac{L}{\pi v}\int_0^{\omega_D} d\omega \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1},$$

for only one polarization type (1 LA). Then the total energy can be written as

$$\begin{aligned} U &= \frac{\hbar L}{\pi v}\int_0^{\omega_D} d\omega \frac{\omega}{e^{\beta\hbar\omega} - 1} \\ &= \frac{\hbar L}{\pi v}\left(\frac{k_B T}{\hbar}\right)^2 \int_0^{\Theta/T} dx \frac{x}{e^x - 1} \end{aligned}$$

where $x = \beta\hbar\omega$, $k_B\Theta = \hbar\omega_D$

We note that

$$N = \int_0^{\omega_D} d\omega D(\omega) = \int_0^{\omega_D} d\omega \frac{L}{\pi v} = \frac{L\omega_D}{\pi v} = \frac{L\hbar\omega_D}{\pi\hbar v} = \frac{Lk_B\Theta}{\pi\hbar v},$$

Thus we have

$$\frac{U}{N} = \frac{\pi\hbar v}{Lk_B\Theta}\frac{\hbar L}{\pi v}\left(\frac{k_B T}{\hbar}\right)^2 \int_0^{\Theta/T} dx \frac{x}{e^x - 1}$$
$$= k_B T\left(\frac{T}{\Theta}\right) \int_0^{\Theta/T} dx \frac{x}{e^x - 1}$$

In the low temperature limit, we have

$$\int_0^{\infty} dx \frac{x}{e^x - 1} = \frac{\pi^2}{6},$$

$$U = \frac{\pi^2}{6} Nk_B T\left(\frac{T}{\Theta}\right)$$

In the high temperature limit

$$\frac{U}{N} = Nk_B T$$

since

$$\frac{x}{e^x - 1} \approx 1.$$

(c) The heat capacity

The heat capacity is

$$C = \frac{\partial U}{\partial T} = \frac{\pi^2}{3} N k_B \left(\frac{T}{\Theta} \right)$$

The entropy is calculated as

$$S = \int \frac{C}{T} dT$$
$$= \frac{\pi^2}{3} N k_B \left(\frac{T}{\Theta} \right)$$

2. Exact expression of the heat capacity for the 1D system

$$U = \frac{\hbar L}{\pi v} \int_0^{\omega_D} d\omega \frac{\omega}{e^{\beta\hbar\omega} - 1}$$

$$C = \frac{d\beta}{dT} \frac{\partial U}{\partial \beta} = \frac{1}{k_B T^2} \frac{\hbar^2 L}{\pi v} \int_0^{\omega_D} d\omega \frac{\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$

$$\frac{C}{N} = \frac{\pi\hbar v}{L k_B \Theta} \frac{1}{k_B T^2} \frac{\hbar^2 L}{\pi v} \int_0^{\omega_D} d\omega \frac{\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}$$
$$= \frac{1}{k_B{}^2 T^2} \frac{\hbar^3}{\Theta} \left(\frac{k_B T}{\hbar} \right)^3 \int_0^{\Theta/T} dx \frac{x^2 e^x}{(e^x - 1)^2}$$
$$= \frac{1}{k_B{}^2 T^2} \frac{\hbar^3}{\Theta} \left(\frac{k_B T}{\hbar} \right)^3 \int_0^{\Theta/T} dx \frac{x^2 e^x}{(e^x - 1)^2}$$

or

$$C = N k_B \left(\frac{T}{\Theta} \right) \int_0^{\Theta/T} dx \frac{x^2 e^x}{(e^x - 1)^2}$$

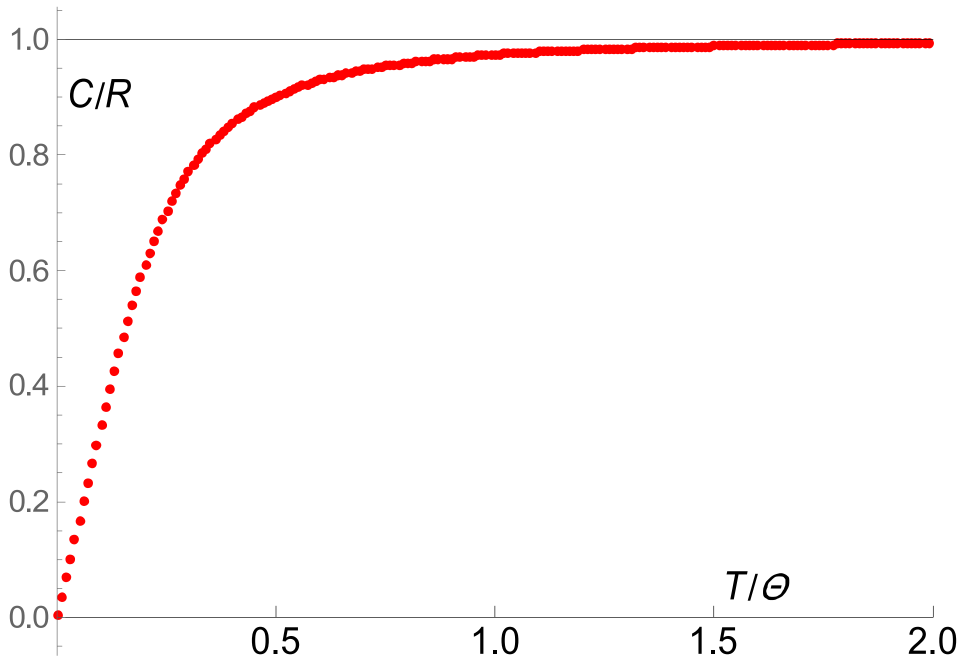

Fig. Plot of the phonon heat capacity (C/R) as a function of T/Θ for the 1D system.

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