Heat capacity of d-dimesional system

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Here we discuss the heat capacity of the system with d-dimension.

1. (Solid State Physics)

(a) Show that in a *d*-dimensional harmonic crystal, the low-frequency density of states varies as ω^{d-1}.

(b) Deduce from this that the low-temperature heat capacity of a harmonic crystal vanishes as T^d in *d* dimensions.

(c) Show that if it should happen that the normal mode frequencies did not vanish linearly with *k* (the wave number) but as k^ν, then the low-temperature heat capacity would vanish as $T^{d/\nu}$.

((**Solution**))

(a) Density of states for *d*-dimensions,

$$D(\omega)d\omega \propto \frac{L^d}{(2\pi)^d} k^{d-1} dk$$

Since $\omega = vk$ (the dispersion relation), we get

$$D(\omega)d\omega \approx \left(\frac{\omega}{v}\right)^{d-1} d\left(\frac{\omega}{v}\right) \approx \omega^{d-1} d\omega$$

Thus $D(\omega)$ is proportional to ω^{d-1}.

(b) The total energy *U* is given by

$$\begin{aligned} U &= \int d\omega D(\omega) < n > \hbar\omega \\ &\approx \int d\omega \omega^{d-1} \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \\ &\approx \int d\omega \frac{\omega^d}{e^{\beta\hbar\omega} - 1} \end{aligned}$$

We put

$$x = \beta\hbar\omega = \frac{\hbar\omega}{k_B T}, \qquad x_D = \beta\hbar\omega_D = \frac{\Theta}{T}$$

So that

$$U \approx T^{d+1} \int_0^{\Theta/T} dx \frac{x^d}{e^x - 1}$$

For $T << \Theta$, we have

$$U \approx T^{d+1} \int_0^{\infty} dx \frac{x^d}{e^x - 1} \approx T^{d+1}$$

Then the heat capacity is obtained as

$$C = \frac{\partial U}{\partial T} \approx T^d$$

(c) Suppose that $\omega \approx k^\nu$ (the dispersion relation). Then we get

$$k \approx \omega^{1/\nu}, \qquad dk \approx \frac{1}{\nu}\omega^{1/\nu - 1}$$

$$D(\omega)d\omega \propto k^{d-1}dk \approx \left(\omega^{1/\nu}\right)^{d-1}\frac{1}{\nu}\omega^{1/\nu-1} \approx \omega^{d/\nu-1}d\omega$$

Thus $D(\omega)$ is proportional to $\omega^{d/\nu-1}$. The total energy U is given by

$$\begin{aligned} U &= \int d\omega D(\omega) < n > \hbar\omega \\ &\approx \int d\omega \omega^{\frac{d}{\nu}-1} \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \\ &\approx T^{\frac{d}{\nu}+1} \int_0^{\Theta/T} dx \frac{d^{d/\nu}}{e^x - 1} \end{aligned}$$

For $T << \Theta$, we have

$$U \approx T^{\frac{d}{\nu}+1}\int_0^\infty dx \frac{x^{d/\nu}}{e^x - 1} \approx T^{\frac{d}{\nu}+1}$$

Then the heat capacity is obtained as

$$C = \frac{\partial U}{\partial T} \approx T^{d/\nu}$$

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2. Example Phonon heat capacity of 2D system

(a) Consider a dielectric crystal made of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^2. (b) Suppose instead, as in many layer structures, that adjacent layers are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures?

Kittel: Introduction to Solid State Physics, seventh edition (John Wiley,1996). Problem 5-4

((**Solution**))

<u>Density of states:</u>

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

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

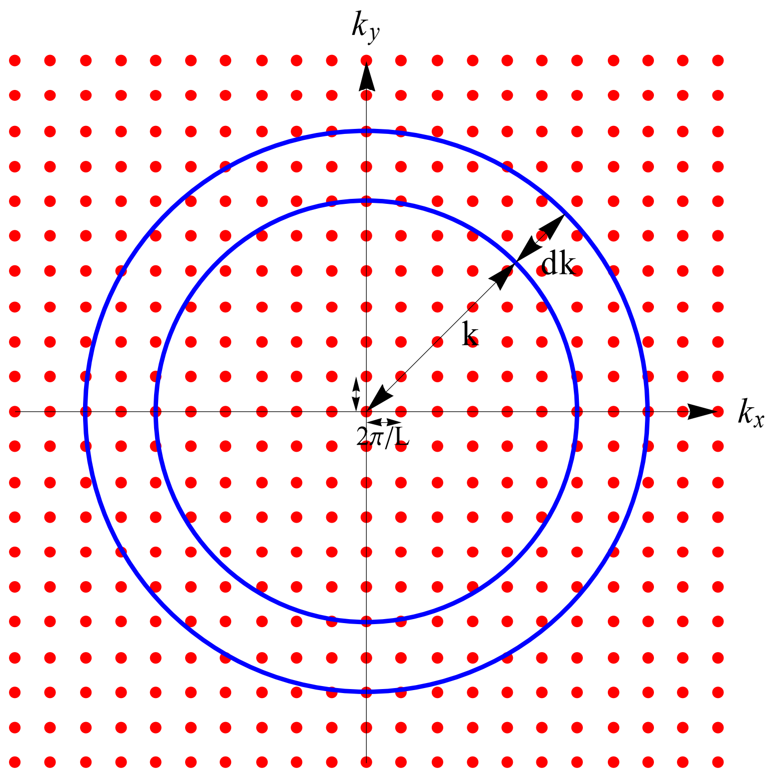
states per unit area of 2D $\boldsymbol{k}$ space, for each polarization (each branch). The density of states is defined by

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

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

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

which is proportional to ω.



(a)

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.

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 transverse acoustic, 1 LA longitudinal acoustic). For simplicity, we assume that the phonon velocity is independent of the polarization ($v_t = v_l = v$). Then we get

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

where the factor 2 comes from two branches, and $x = \beta\hbar\omega$ and $k_B\Theta = \hbar\omega_D$

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 get

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

leading to the expression

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

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

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

The heat capacity

The heat capacity is

$$C = \frac{\partial U}{\partial T} = 24\varsigma(3) N k_B \left(\frac{T}{\Theta}\right)^2 = 28.8492 N k_B \left(\frac{T}{\Theta}\right)^2 \qquad \text{at low temperatures}$$

$$C = \frac{\partial U}{\partial T} = 2k_B N \qquad \text{or} \qquad C = 2N_A k_B = 2R$$

Entropy

The entropy is calculated as

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

(b) If the layers are weakly bound together, the system behaves as a linear structure with each plane as a vibrating unit. By induction from the results for 2D and 3D systems, we expect

$$C \propto T$$

But this only holds at extremely low temperatures such that

$$k_B T << \hbar\omega_D \approx \frac{\hbar v N_{layer}}{L}$$

where $\frac{N_{layer}}{L}$ is the number of layers per unit length.

((Note))

In this case, since the coupling in between layers are weaker than the coupling inside the layers, at extremely low temperatures, the degrees of freedom for the motion inside the layers will be frozen, and the motion of the atoms is restricted in the direction perpendicular to the layers.

Therefore the system becomes 1-D. Follow a similar calculation as in part (a), we can find the heat capacity for 1-D system in low temperature will be proportional to T.

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3. Heat capacity of 1D system

The density of state for the 1D system is

$$D(\omega)d\omega = \left(\frac{L}{2\pi}\right)2dk = \frac{L}{\pi}dk = \frac{L}{\pi v}d\omega$$

There is only the longitudinal mode for the 1D system. The factor $2dk$ comes from the fact that the dispersion relation is an even function of k. The internal energy U for each branch is

$$U = \int D(\omega)d\omega \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}$$

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

We introduce a new parameter,

$$x = \beta\hbar\omega, \qquad dx = \beta\hbar d\omega$$

$$\beta\hbar\omega_D = \frac{k_B\Theta}{k_B T} = \frac{\Theta}{T}$$

Then we have

$$U = \frac{L}{\pi v}\frac{k_B{}^2T^2}{\hbar}\int_0^{\Theta/T} dx \frac{x}{e^x-1}$$

We note that

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

or

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

Thus we have

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

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

or

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

In the low temperature limit $(T << \Theta)$,

$$U = Nk_BT\left(\frac{T}{\Theta}\right)\int_0^{\infty} dx\frac{x}{e^x-1} = \frac{\pi^2}{6}Nk_BT\left(\frac{T}{\Theta}\right)$$

where

$$\int_0^{\infty} dx\frac{x}{e^x-1} = \frac{\pi^2}{6} = 1.64493$$

The heat capacity is

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

which is proportional to T as is expected. In the high temperature limit $(T >> \Theta)$,

$$U \approx Nk_BT\left(\frac{T}{\Theta}\right)\int_0^{\Theta/T} dx = Nk_BT$$

The heat capacity is

$$C = \frac{\partial U}{\partial T} = Nk_B \qquad \text{or} \qquad C = N_Ak_B = R$$