

Problem 7.1 Volume change under deformation

As the displacement gradient $u_{\alpha\beta}$ is a real symmetric rank-2 tensor, it can be diagonalised by an orthogonal transformation. We hence consider a small cube of the material that is oriented along the tensor's eigenvectors. Under the deformation u , this cube is only elongated or compressed along the axes, i.e. there is no shear strain. If the cube's original volume (i.e. without deformation) is $V = L^3$, with L small enough that the deformation over the extent of the cube can be approximated by a linear Taylor expansion of u , the deformation changes the cube's volume to

$$V + \delta V = \left(L + \frac{\partial u_x}{\partial x} L\right) \left(L + \frac{\partial u_y}{\partial y} L\right) \left(L + \frac{\partial u_z}{\partial z} L\right) \quad (1)$$

$$= V \left(1 + \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} + \mathcal{O}(u_{\alpha\beta}^2)\right). \quad (2)$$

Then

$$\frac{\delta V}{V} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \equiv \operatorname{div} \mathbf{u}. \quad (3)$$

Problem 7.2 Quantum corrections to classical specific heat

Starting from the general definition of the specific heat for phonons with dispersion $\omega_{\vec{k}}$,

$$c_V = \frac{1}{V} \frac{\partial E}{\partial T} = \frac{1}{V} \sum_{\vec{k}} \frac{\partial}{\partial T} \frac{\hbar\omega_{\vec{k}}}{e^{\beta\hbar\omega_{\vec{k}}} - 1}, \quad (4)$$

we expand the fraction in $\beta\hbar\omega_{\vec{k}} = \hbar\omega_{\vec{k}}/k_B T \ll 1$ (cf. the lecture notes):

$$c_V = \frac{1}{V} \sum_{\vec{k}} \frac{\partial}{\partial T} \hbar\omega_{\vec{k}} \frac{1}{\beta\hbar\omega_{\vec{k}}} \left(1 - \frac{\beta\hbar\omega_{\vec{k}}}{2} + \frac{(\beta\hbar\omega_{\vec{k}})^2}{12} + \dots\right) \quad (5)$$

$$= \frac{1}{V} \sum_{\vec{k}} \frac{\partial}{\partial T} \left[k_B T \left(1 - \frac{\hbar\omega_{\vec{k}}}{2k_B T} + \frac{(\hbar\omega_{\vec{k}})^2}{12(k_B T)^2} + \mathcal{O}\left(\left(\frac{\hbar\omega_{\vec{k}}}{k_B T}\right)^3\right)\right) \right] \quad (6)$$

$$= \frac{k_B}{V} \sum_{\vec{k}} \left(1 - \frac{(\hbar\omega_{\vec{k}})^2}{12(k_B T)^2} + \mathcal{O}\left(\left(\frac{\hbar\omega_{\vec{k}}}{k_B T}\right)^3\right)\right) \quad (7)$$

According to the Debye model we approximate the dispersion $\omega_{\vec{k}} = ck$ and replace the sum over modes by an integration over a momentum sphere with radius k_D :

$$\sum_{\vec{k}} \rightarrow \sum_s V \int \frac{d^3k}{(2\pi)^3} \rightarrow \frac{3V}{2\pi^2} \int_0^{k_D} dk k^2, \quad (8)$$

where we have accounted for the fact that in 3D there are three phonon branches s . Then, neglecting corrections of order $\mathcal{O}((\theta_D/T)^3)$,

$$c_V = \frac{3k_B}{2\pi^2} \int_0^{k_D} dk k^2 - \frac{(\hbar c)^2}{8\pi^2 k_B T^2} \int_0^{k_D} dk k^4 \quad (9)$$

$$= \frac{k_B k_D^3}{2\pi^2} - \frac{(\hbar c)^2 k_D^5}{40\pi^2 k_B T^2}. \quad (10)$$

Using $k_D^3 = 6\pi^2 N/V$ and $(\hbar ck_D)^2 = (k_B \theta_D)^2$, we finally arrive at

$$c_V = \frac{3k_B N}{V} \left[1 - \frac{1}{20} \left(\frac{\theta_D}{T} \right)^2 \right], \quad (11)$$

where the first term is the Dulong-Petit law and the second one the leading high-temperature correction.

Problem 7.3 Specific heat in d dimensions

Let us start from the phonon energy of a d -dimensional crystal:

$$E = \sum_s \int \frac{d^d k}{(2\pi)^d} \frac{\hbar \omega_{\vec{k}}} {e^{\beta \hbar \omega_{\vec{k}}} - 1}. \quad (12)$$

For low temperatures we can restrict the sum to the acoustic phonon branches and linearise their dispersion $\omega_{s,\vec{k}} = c_s(\hat{k})k$, with a sound velocity c_s that in general depends on the direction \hat{k} . Then, for $d = 2$ dimensions, we can go to polar coordinates $\vec{k} \rightarrow (k, \phi)$ and extend the integration region to infinity:

$$E = \sum_s \int_0^{2\pi} \frac{d\phi}{(2\pi)^2} \int_0^\infty dk \frac{\hbar c_s(\phi) k^2}{e^{\beta \hbar c_s(\phi) k} - 1}. \quad (13)$$

Then, substituting

$$x = \beta \hbar c_s(\phi) k, \quad (14)$$

we have

$$E = \sum_s \int_0^{2\pi} \frac{d\phi}{(2\pi)^2} \frac{\hbar c_s(\phi)}{(\beta \hbar c_s(\phi))^3} \int_0^\infty dx \frac{x^2}{e^x - 1}. \quad (15)$$

The integral on the right is

$$\int_0^\infty dx \frac{x^2}{e^x - 1} = 2 \sum_{n=1}^\infty \frac{1}{n^3} = 2\zeta(3), \quad (16)$$

with the Riemann Zeta function $\zeta(3) \approx 1.202$. Furthermore, we define the effective sound velocity

$$\frac{1}{\bar{c}^2} = \frac{1}{2} \int_0^{2\pi} \frac{d\phi}{2\pi c_s(\phi)^2}, \quad (17)$$

which, for an isotropic crystal, reduces to

$$\frac{1}{\bar{c}^2} = \frac{1}{2} \left(\frac{1}{c_l^2} + \frac{1}{c_t^2} \right). \quad (18)$$

Then we have for the energy

$$E = \frac{2\zeta(3)}{\pi (\hbar \bar{c})^2} (k_B T)^3 \quad (19)$$

and thus the specific heat

$$c_V = \frac{1}{V} \frac{\partial E}{\partial T} = \frac{6\zeta(3)k_B}{\pi(\hbar\bar{c})^2} (k_B T)^2 \quad (20)$$

is proportional to the square of the temperature.

Generalising our analysis to d dimensions, one notices that the momentum integral in Eq. (12) will contain the d -th power of the momentum k , because the integral measure $d^d k \sim k^{d-1}$ and the dispersion $\omega_{\vec{k}}$ is linear in k . The substitution (14) will therefore produce a temperature dependence of the energy

$$E \sim T^{d+1}, \quad (21)$$

so that the specific heat

$$c_V \sim T^d \quad (22)$$

contains the dimensionality as the power of the temperature dependence.

This is in contrast to the specific heat of electrons in a metal, which is linear in temperature, independently of the system's dimensionality. The reason for this difference is the presence of a Fermi sea with an extended Fermi surface, which provides a large, and to leading order temperature-independent, density of states at the Fermi level.

On the other hand, the specific heat of phonons in two dimensions, Eq. (20), is very similar to the expression we found for graphene in problem 6.1, cf. Eq. (46) of the corresponding solution sheet. The main difference between a metal and graphene is that, while both are fermionic systems, in the former the density of states is finite at the Fermi level due to the presence of an extended Fermi surface, whereas $N(\mu) = 0$ in graphene, where the Fermi level is pinned to the Dirac points. Therefore, the number of thermally excited quasiparticles in a metal is, to leading order, $\sim N(\mu)T$, in contrast to graphene, where this term vanishes. Here, the density of states around the Fermi level grows linearly $N(\varepsilon) \propto \varepsilon$ such that the number of excitations, and hence the heat capacity, goes as $\sim \int_0^T d\varepsilon N(\varepsilon) \propto T^2$. The density of states for the two-dimensional phonon system has the same form $N(\varepsilon) \propto \varepsilon$, explaining the identical result for the specific heat, up to numeric factors due to mode counting and the replacement $\bar{c} \rightarrow v_F$.