Institute of Theoretical Physics
University of Cologne
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Solid State Theory

Exercise sheet 3

This exercise sheet will be discussed on Friday, December 2nd 2022.
You should hand in your solution of the exercise marked with (★)
via mail (gresista@thp.uni-koeln.de) by 10:00 AM on Thursday, December 1st 2022.

Exercise sheets online at `www.thp.uni-koeln.de/trebst/Lectures/2022-SolidState.shtml`

1 Specific heat of phonons (★)

The goal of this exercise is to study the contribution of phonons to the specific heat of a crystal. To this end, let us consider the phonon Hamiltonian in the harmonic approximation

$$H_{ph} = \sum_{\boldsymbol{k}\in 1.\mathrm{BZ}; n=1,2,\dots,d\,r} \hbar\omega_n(\boldsymbol{k}) \left(b^\dagger_{\boldsymbol{k},n} b_{\boldsymbol{k},n} + \frac{1}{2} \right) \tag{1}$$

with $b^\dagger_{\boldsymbol{k},n}$ and $b_{\boldsymbol{k},n}$ being bosonic creation and annihilation operators, respectively, $n = 1, 2, ..., d\,r$ labels the phonon branches for r ions per unit cell in d dimensions, and $\omega_n(\boldsymbol{k})$ denote the energy dispersions.
The average occupation number of a phonon mode at temperature $T \geq 0$ is given by the Bose-Einstein distribution function ($\beta = \frac{1}{k_B T}$)

$$n_B(\hbar\omega_n(\boldsymbol{k})) \equiv \langle b^\dagger_{\boldsymbol{k},n} b_{\boldsymbol{k},n} \rangle = \frac{1}{e^{\beta\hbar\omega_n(\boldsymbol{k})} - 1}.$$

The thermal average is defined via $\langle \hat{O} \rangle = \frac{\mathrm{Tr}\left(e^{-\beta\hat{H}}\hat{O}\right)}{Z}$, where $Z = \mathrm{Tr}\left(e^{-\beta\hat{H}}\right)$ is the partition function. We want to calculate the specific heat C given by

$$C(T) = \frac{\partial \langle \hat{H} \rangle}{\partial T}.$$

a) Show that

$$C(T) = \frac{\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2}{k_B T^2},$$

i.e. that the specific heat is a measure of *variations* in energy

High-temperature limit:
The phonon dispersions are bounded from above with a maximum value $\omega_{\max} \equiv \max\limits_{n,\boldsymbol{k}}\{\omega_n(\boldsymbol{k})\}$.

b) Show that for high temperatures $T \gg \hbar\omega_{\max}/k_B$, the specific heat follows the *law of Dulong-Petit* and is given by the constant value

$$C\left(T \gg \hbar\omega_{\max}/k_B\right) = d\,r\,k_B\,N,$$

where N is the number of unit cells.

Phonon density of states:
It is convenient to write the specific heat in the form

$$C(T) = d\,r\,k_B\,N \int_0^\infty d\varepsilon\, g(\varepsilon)\, \frac{(\beta\varepsilon)^2 e^{\beta\varepsilon}}{(e^{\beta\varepsilon} - 1)^2}, \tag{2}$$

where $g(\varepsilon)$ is the phonon density of states:

$$g(\varepsilon) = \frac{1}{drN} \sum_{\boldsymbol{k} \in 1.\mathrm{BZ}; n=1,2,\ldots d\, r} \delta(\varepsilon - \hbar\omega_n(\boldsymbol{k})). \tag{3}$$

c) Evaluate the integral $\int_0^\infty d\varepsilon g(\varepsilon)$ to show the density of states in normalised.

Low-temperature limit:
The energy of the optical branches is also bounded from below with a minimum value $\omega_{\min}^{\mathrm{opt}} \equiv \min\limits_{n,\boldsymbol{k}}\{\omega_n(\boldsymbol{k}) | \omega_n \text{ optical}\}$.
At low temperatures $k_B T \ll \hbar\omega_{\min}^{\mathrm{opt}}$, the phonon density of states is solely determined by the d acoustic phonon branches. Their dispersions assume the form $\omega_j(\boldsymbol{k}) = v_{s,j}(\hat{\boldsymbol{k}})|\boldsymbol{k}|$ with $j = 1, ..., d$. In general, these sound velocities $v_{s,j}(\hat{\boldsymbol{k}})$ depend on $\hat{\boldsymbol{k}} = \boldsymbol{k}/|\boldsymbol{k}|$. In the following calculation assume the velocites are isotropic $v_{s,j}(\hat{\boldsymbol{k}}) = v_s$ for simplicity. Additionally assume continuous $\mathbf{k}$ values and replace the corresponding sum by an integral.

d) Evaluate the phonon specific heat, Eq. (2), at low temperatures to show that

$$C\left(T \ll \hbar\omega_{\min}^{\mathrm{opt}}/k_B\right) \sim T^d. \tag{4}$$

Hints: Show that $g(\varepsilon \ll \hbar\omega_{\min}^{\mathrm{opt}}) \sim \varepsilon^{d-1}$ and subsitute $\varepsilon = k_B T x$ in Eq. (2).

e) Calculate the prefactor in $d = 3$ dimensions. *Hint:* $\int_0^\infty dx \, \frac{x^4 \, e^x}{(e^x-1)^2} = \frac{4\pi^4}{15}$

2 Debye model

In order to describe the crossover between the low- and high-temperature limits, one often uses the Debye model. Here, the phonon density of states is assumed to have the form

$$g_D(\varepsilon) = d\frac{\varepsilon^{d-1}}{\varepsilon_D^d}\Theta(\varepsilon_D - \varepsilon), \tag{5}$$

where ε_D is the *Debye energy*, which also defines the *Debye temperature* $T_D = \varepsilon_D/k_B$.

a) Show that this density of state is correctly normalised by evaluating the integral $\int_0^\infty d\varepsilon g_D(\varepsilon)$.

b) Confirm that the expression Eq. (2) for the specific heat with the Debye density of states Eq. (5) indeed recovers the Dulong-Petit law at high temperatures and the behavior $C \sim T^d$ at low temperatures.

c) Compare the result in the low-temperature regime for $d = 3$ with the result obtained in the final task of the previous exercise and use this to derive an explicit formula for ε_D.