Institute for Theoretical Physics
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Solid State Theory

Problem set 3

Winter Term 2016

Website: `http://www.thp.uni-koeln.de/trebst/Lectures/2016-SolidState.shtml`
Due date: Discussed in class on **Thursday, December 1st**.

If you turn in your solutions by Wednesday noon (November 30th), they will be graded.
Please submit your solutions to Henry Legg at hlegg@uni-koeln.de.

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

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

with $b^\dagger_{\mathbf{k},n}$ and $b_{\mathbf{k},n}$ being bosonic creation and annihilation operators, respectively, $n = 1, 2, \ldots, d\,r$ labels the phonon branches for r ions per unit cell in d dimensions, and $\omega_n(\mathbf{k})$ 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 ($\beta = \frac{1}{k_B T}$)

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

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. The quantity of interest is the specific heat C given by

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

- Show that

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

- *High-temperature limit:* The phonon dispersions are bounded from above with a maximum value $\omega_{\max} \equiv \max_{n,\mathbf{k}}\{\omega_n(\mathbf{k})\}$. Show that for temperatures $T \gg \hbar\omega_{\max}/k_B$, the specific heat follows the *law of Dulong-Petit* and is given by the constant value

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

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:

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

Evaluate the integral $\int_0^\infty d\varepsilon g(\varepsilon)$.

- *Low-temperature limit:* The energy of the optical branches is also bounded from below with a minimum value $\omega_{\min}^{\mathrm{opt}} \equiv \min\limits_{n,\mathbf{k}}\{\omega_n(\mathbf{k})|\omega_n \text{ optical}\}$.

  At low temperatures $k_BT \ll \hbar\omega_{\min}^{\mathrm{opt}}$, the phonon density of states is solely determined by the d acoustic phonon branches. Their dispersions assume the form $\omega_j(\mathbf{k}) = v_{s,j}(\hat{\mathbf{k}})|\mathbf{k}|$ with $j = 1,\ldots,d$. The sound velocities $v_{s,j}(\hat{\mathbf{k}})$ only depend on $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$. Evaluate the phonon specific heat, Eq. (2), at low temperatures to show that

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

  Hint: Show that $g(\varepsilon \ll \hbar\omega_{\min}^{\mathrm{opt}}) \sim \varepsilon^{d-1}$ and subsitute $\varepsilon = k_BTx$ in Eq. (2).
  Calculate the prefactor in $d = 3$ dimensions for constant sound velocities $v_{s,j}(\hat{\mathbf{k}}) \equiv v_s$.
  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

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

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

- Show that this density of state is correctly normalized by evaluating the integral $\int_0^\infty d\varepsilon g_D(\varepsilon)$.
- Comfirm that the expression (2) for the specific heat with the Debye density of states (5) indeed recovers the Dulong-Petit law at high temperatures and the behavior $C \sim T^d$ at low temperatures.
- Compare the result in the low-temperature regime for $d = 3$ with the result obtained in **2**.d) to derive an explicit formula for ε_D.