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Theoretical Condensed Matter Physics
Exercise 7

(Submission: 14.12.18, discussion: 17./19.12.18)

7.1 Einstein model (optical phonons) (8 points)

According to classical physics, the heat capacity of solids follows the *Dulong-Petit law*. It stipulates that, by the equipartition theorem of classical statistical mechanics, the heat capacity should be independent of the temperature. Experimentally, however, one finds that the heat capacity of solids decreases when the temperature is lowered. In 1907, using the then new ideas of early quantum theory, Einstein was the first to point towards a resolution of this conflict.

Consider a three-dimensional solid composed of N atoms. Assume that each atom can be described as a quantum harmonic oscillator of frequency Ω, vibrating *independently* of all other atoms. This independence is the crucial assumption in Einstein's simplified model.

a) Calculate the *canonical* partition function $Z = \mathrm{Tr}\, \mathrm{e}^{-\beta \hat{H}}$ for a single quantum oscillator of frequency Ω.

b) From the partition function for the single oscillator, obtain the internal energy for the whole system

$$\langle H \rangle = U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta}, \tag{1}$$

and the total heat capacity

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V . \tag{2}$$

c) Write C_V in terms of the so-called *Einstein temperature* $\Theta_E = \hbar\Omega/k_B$, and compare both the high- and low-temperature limits with the experimentally observed scalings:

$$C_V^{\text{exp.}} = \begin{cases} 3Nk_B, & T \to \infty, \\ \gamma T + AT^3, & T \to 0. \end{cases} \tag{3}$$

For high T, this is the Dulong-Petit law. In the low-temperature limit, electrons give a contribution linear in T (hence, for an insulator, $\gamma = 0$), while phonons contribute with T^3. Does the Einstein model fully resolve the low-temperature problem with the classical heat capacity?

7.2 Debye model (acoustic phonons) (12 points)

A more realistic model, introduced by Debye, can appropriately account for low-lying acoustic phonon branches. In this model, it is considered that each of the acoustic phonon branches, labeled by the quantum number n, obeys a linear dispersion

$$\varepsilon_{n,\boldsymbol{k}} = \hbar\,\omega_{n,\boldsymbol{k}} = \hbar\,c_n\,|\boldsymbol{k}|, \tag{4}$$

with $n = 1, \ldots d$, where d is the spatial dimensionality. We will assume that our solid is isotropic and hence the sound speed c_n is the same for all modes.

a) Use Eq. (4) to calculate the density of states $\mathcal{D}(\varepsilon)$ for the Debye model in $d = 1$, 2 and 3 dimensions,

$$\mathcal{D}(\varepsilon) = \frac{1}{V}\sum_{n,\boldsymbol{k}} \delta\left(\varepsilon - \varepsilon_{n,\boldsymbol{k}}\right).$$

What is the total number of phonon modes per branch N_{ph}? Accordingly, introduce a cut-off frequency ω_D in $\mathcal{D}(\varepsilon)$, known as the *Debye frequency*, to obey this total number of modes. Rewrite $\mathcal{D}(\varepsilon)$ in terms of ω_D and N_{ph}.

b) Relate qualitatively the Debye temperature $\Theta_D = \frac{\hbar\omega_D}{k_B}$ of phonons with the Fermi level of electrons: What happens for $T > \Theta_D$ and $T < \Theta_D$?

c) Now determine the specific heat $C_V(T)$ using the formula

$$C_V(T) = \frac{\partial}{\partial T}\int_0^{+\infty} d\varepsilon\,\mathcal{D}(\varepsilon)\,\varepsilon\,n_B(\varepsilon),$$

where n_B is the Bose-Einstein distribution function. Why is that distribution function used here? Study the behaviour of C_V at low ($T \to 0$) and high ($T \to \infty$) temperatures and sketch $C_V(T)$.

Hint: $\int_0^{+\infty} du\,u^{d+1}\frac{e^u}{(e^u-1)^2} = \frac{\pi^2}{3}, 6\zeta(3), \frac{4\pi^4}{15}$ for $d = 1, 2, 3$, respectively.