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Condensed Matter Theory 1 — Exercise 5

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To be discussed on: *Thursday 2023/11/30*

1. Specific heat of phonons

Let us consider the phonon Hamiltonian $\mathcal{H}_{ph} \equiv \mathcal{H}$ in the harmonic approximation

$$\mathcal{H} = \sum_{\boldsymbol{k}\in 1.\text{BZ};\, n=1,2,\ldots,d\,r} \hbar\omega_n(\boldsymbol{k}) \left(b^\dagger_{\boldsymbol{k},n} b_{\boldsymbol{k},n} + \frac{1}{2} \right) \ . \tag{1}$$

Here, $b^\dagger_{\boldsymbol{k},n}$ and $b_{\boldsymbol{k},n}$ are the bosonic creation and annihilation operators, respectively. The index $n = 1, 2, ..., d\,r$ labels the phonon branches for r ions per unit cell in d spatial dimensions. $\omega_n(\boldsymbol{k})$ denotes the energy dispersion as function of the momentum $\boldsymbol{k}$. The average occupation number of a phonon mode at temperature T is given by the Bose-Einstein distribution function

$$n_\text{B}(\beta\hbar\omega_n(\boldsymbol{k})) \equiv \langle b^\dagger_{\boldsymbol{k},n} b_{\boldsymbol{k},n} \rangle_{\mathcal{H}} = \frac{1}{e^{\beta\hbar\omega_n(\boldsymbol{k})} - 1} \tag{2}$$

with $\beta = \frac{1}{k_B T}$. The quantity of interest is the specific heat per unit cell C given by

$$C(T) = \frac{\partial E}{\partial T}, \quad \text{with} \quad E = \frac{1}{N} \langle \mathcal{H} \rangle_{\mathcal{H}}, \tag{3}$$

where N is the number of unit cells in the crystal.

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

$$C = d\,r\,k_B \ . \tag{4}$$

b) *Phonon density of states:* Show that the specific heat can be written in the form

$$C = d\,r\,k_B \int_0^\infty d\varepsilon\, g(\varepsilon)\, \frac{(\beta\varepsilon)^2 e^{\beta\varepsilon}}{(e^{\beta\varepsilon} - 1)^2} \ , \tag{5}$$

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

$$g(\varepsilon) = \frac{1}{d\,r\,N} \sum_{\boldsymbol{k}\in 1.\text{BZ};n=1,2,\ldots d\,r} \delta(\varepsilon - \hbar\omega_n(\boldsymbol{k})) \ . \tag{6}$$

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

c) *Diatomic chain:* The dispersion relation $\omega_n(k)$ for the one-dimensional, diatomic chain, that was considered in Sheet 03, consists of two branches ($n = 1, 2$),

$$\omega_{1,2} = \omega_0 \kappa^{-1/2} \left(1 \pm \sqrt{1 - \kappa^2 \sin^2 \frac{ka}{2}} \right)^{1/2}, \tag{7}$$

where the coefficient $0 < \kappa \leq 1$ is determined by the ratio of masses. Show that the density of states can be written in the form

$$g(\varepsilon) = \frac{a}{2\pi\hbar} \sum_{n=1,2} \frac{\Theta(\varepsilon - \omega_n^{\text{min}})\Theta(\omega_n^{\text{max}} - \varepsilon)}{|\omega_n'(k_{0n})|}, \tag{8}$$

where $\Theta(x)$ is Heaviside step function, ω_n^{min} and ω_n^{max} are the minimum and maximum frequency of the n-th branch, respectively, and k_{0n} is determined by the equation $\hbar\omega_n(k_{0n}) = \varepsilon$. How many singular points does the function $g(\varepsilon)$ possess? Compute $g(\varepsilon = 0)$.

d) *Low-temperature limit:* After substituting $\varepsilon = x k_B T$ in Eq. (5), argue that the low-temperature limit of the specific heat is in general governed by the phonon density of states for small energies. At small energies ε, the phonon density of states $g(\varepsilon)$ is solely determined by the d acoustic phonon branches. Also, the acoustic dispersions are approximately given by $\omega_j(\boldsymbol{k}) = c_j|\boldsymbol{k}|$ with $j = 1, ..., d$. Show that $g(\varepsilon) \sim \varepsilon^{d-1}$ for $\varepsilon \to 0$. With the help of this result evaluate the phonon specific heat at low temperatures to show that $C \sim T^d$. Calculate the prefactor in $d = 3$ dimensions for constant sound velocities $c_j(\hat{\boldsymbol{k}}) \equiv c$ and in $d = 2$ dimensions for the two-dimensional triangular lattice considered in Sheet 04 (use the sound velocities obtained in 1e).
Hint: $\int_0^\infty dx \, \frac{x^4 \, e^x}{(e^x-1)^2} = \frac{4\pi^4}{15}$*;* $\int_0^\infty dx \, \frac{x^3 \, e^x}{(e^x-1)^2} = 6\zeta(3)$*, where* $\zeta(x)$ *is Riemann zeta-function.*

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

$$g_D(\varepsilon) = \frac{d \, \varepsilon^{d-1}}{\varepsilon_D^d} \Theta(\varepsilon_D - \varepsilon), \tag{9}$$

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 states is correctly normalized by evaluating the integral $\int_0^\infty d\varepsilon g_D(\varepsilon)$.

b) Confirm that the expression (5) for the specific heat with the Debye density of states (9) indeed recovers the Dulong-Petit law at high temperatures and the behavior $C \sim T^d$ at low temperatures.

3. Kronig–Penney model

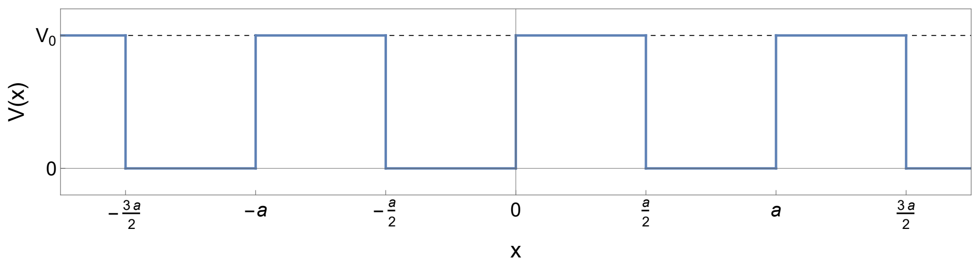

Figure 1: The periodic potential $V(x)$.

Consider a periodic rectangular potential with periodicity a and strength V_0 as shown in Fig. 1,

$$V(x) = \begin{cases} V_0 & x \in [na, na + \frac{a}{2}) \\ 0 & x \in [na - \frac{a}{2}, na) \end{cases} \quad (n \in \mathbb{Z}) \ . \tag{10}$$

We want to solve the Schrödinger equation

$$\left(-\frac{\hbar^2 \partial_x^2}{2m} + V(x) \right) \Psi(x) = E\, \Psi(x) \tag{11}$$

in order to determine the band structure. According to Bloch's theorem,

$$\Psi_{nk}(x) = e^{ikx} u_{nk}(x), \quad \text{with } u_{nk}(x) = u_{nk}(x + ma) \text{ for all } m \in \mathbb{Z}, \tag{12}$$

it is sufficient to solve problem only in one period of the potential, for example $x \in [-a/2, a/2]$.

a) *Exact solution, part 1/2:* Show that the ansatz

$$\Psi_I(x) \quad = Ae^{i\alpha x} + Be^{-i\alpha x} \quad (0 < x < a/2) \tag{13}$$
$$\Psi_{II}(x) \quad = Ce^{i\beta x} + De^{-i\beta x} \quad (-a/2 < x < 0) \tag{14}$$

where $\alpha = \frac{\sqrt{2m(E-V_0)}}{\hbar}$ and $\beta = \frac{\sqrt{2mE}}{\hbar}$ solves the Schrödinger equation in the respective range. At the origin $x = 0$ the following conditions must be obeyed

$$\Psi_I(0) \quad = \quad \Psi_{II}(0) \ , \tag{15}$$
$$\Psi_I'(0) \quad = \quad \Psi_{II}'(0) \ . \tag{16}$$

Furthermore, in order to comply with Bloch's theorem, the boundary conditions at $x = \pm a/2$ are

$$u_I(a/2) \quad = \quad u_{II}(-a/2) \ , \tag{17}$$
$$u_I'(a/2) \quad = \quad u_{II}'(-a/2) \ . \tag{18}$$

Write the four conditions in the form of a matrix equation

$$\boldsymbol{M}(E,k) \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{19}$$

and determine $\boldsymbol{M}(E,k)$. A non-trivial solutions exists if its determinant vanishes

$$\det \boldsymbol{M}(E,k) \stackrel{!}{=} 0 \tag{20}$$

b) *Exact solution, part 2/2:* Show that Eq. (20) is equivalent to

$$\cos(ak) = \cos(\frac{a\,\alpha}{2})\,\cos(\frac{a\,\beta}{2}) - \frac{\alpha^2+\beta^2}{2\,\alpha\beta}\sin(\frac{a\,\alpha}{2})\,\sin(\frac{a\,\beta}{2})\ . \tag{21}$$

This equation can not be solved analytically for the dispersion $E(k)$. Visualize the electronic dispersion relation $E(k)$ by plotting its inverse $k(E)$.
Hint: For simplicity, set $a, \hbar, m,$ and V_0 to 1.

c) *Perturbation theory:* Start from the eigenstates of the free Hamiltonian H_0

$$H_0\,|p\rangle = E_p\,|p\rangle = \frac{\hbar^2 k^2}{2m}\,|p\rangle \tag{22}$$

with $\langle x|\,p\rangle = e^{ipx}/\sqrt{2\pi}$. Treat the effect of the periodic potential H_1 with matrix elements $\langle x|\,H_1\,|x'\rangle = V(x)\delta_{x,x'}$ in perturbation theory. To do so, show that the matrix elements of the periodic potential in momentum space are given by

$$\langle p|\,H_1\,|p'\rangle = V_0 \sum_{m=-\infty}^{\infty} \frac{e^{i\pi m}-1}{2\pi i m}\delta_{p-p',\frac{2\pi\,m}{a}} \tag{23}$$

There is an overall energy shift $\langle p|\,H_1\,|p\rangle = V_0/2$. Identify the points within the 1. BZ where the unperturbed spectrum is degenerate. Apply degenerate perturbation theory in lowest order in the periodic potential in order to calculate the band gaps. Show that in this approximation the n^{th} band gap with $n = 1, 2, 3, ...$ is given by

$$\Delta_n = \begin{cases} \frac{2\,V_0}{\pi n}, & n \text{ odd} \\ 0, & n \text{ even} \end{cases}\ , \tag{24}$$

i.e., only every second degeneracy is lifted. Sketch the result in the reduced zone scheme. In which limit does perturbation theory yield a good approximation for the spectrum $E(k)$?