Solid State Theory

Priv.-Doz. Dr. R. Bulla, K. Duivenvoorden

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Sheet 5: return on: Monday, Dec 10, 2012, 12:00 (SR THP)

Exercise 1: Discrete vs. continuous functions

Consider a sequence of functions $\rho_{\Lambda}(\varepsilon)$, each function given as an infinite sum of δ -peaks at energies $\varepsilon_{n,\Lambda}$ with weights $a_{n,\Lambda}$:

$$\rho_{\Lambda}(\varepsilon) = \sum_{n=1}^{\infty} a_{n,\Lambda} \,\delta(\varepsilon - \varepsilon_{n,\Lambda}) \;,$$

with

$$\varepsilon_{n,\Lambda} = \frac{1}{2}\Lambda^{-n}(\Lambda+1) , \ a_{n,\Lambda} = \Lambda^{-n}(\Lambda-1) ,$$

and $\Lambda > 1$.

a) Calculate the total weight of $\rho_{\Lambda}(\varepsilon)$, that is the integral

$$\int_{-\infty}^{\infty} \mathrm{d}\varepsilon \,\rho_{\Lambda}(\varepsilon) \,\,.$$

(1 points)

For any $\Lambda > 1$, the function $\rho_{\Lambda}(\varepsilon)$ is discrete, although it consists of an infinite number of δ -peaks in the interval]0,1[. A continuous function is obtained in the limit $\Lambda \to 1$:

$$\rho_{\rm c}(\varepsilon) = \lim_{\Lambda \to 1} \rho_{\Lambda}(\varepsilon) \ .$$

b) Calculate the resulting $\rho_{\rm c}(\varepsilon)$ by using a suitable representation of the δ -function:

$$\delta(\varepsilon - \varepsilon_{n,\Lambda}) \to g_{n,\Lambda}(\varepsilon)$$
 .

where $g_{n,\Lambda}(\varepsilon)$ is a constant on a suitable range of ε -values, with a width proportional to Λ^{-n} , and zero elsewhere. (4 points)

c) One might also think of replacing the $g_{n,\Lambda}(\varepsilon)$ as used in b) by Lorentzians of width Λ^{-n} (and proper weight). Show that such a choice leads to a divergence of $\rho_{\rm c}(\varepsilon)$ for $\varepsilon \to 0$. (4 points)

Exercise 2: Density of states

Here we consider phonon branches with general dispersion relations $\omega_j(\vec{q})$.

a) Show that the phonon density of states can be calculated from the dispersion relations via the integral

$$n(\omega) = \frac{V}{N} \sum_{j} \frac{1}{(2\pi)^d} \int_{S(\omega)} \frac{\mathrm{d}s}{|\nabla_{\vec{q}} \,\omega_j(\vec{q})|} ,$$

with $S(\omega)$ the area defined by $\omega_j(\vec{q}) = \omega$, and $\int_{S(\omega)} ds$ the integral over this area. (1 points)

We now focus on the density of states close to a saddle point of the dispersion relation:

$$\omega(\vec{q}) = \omega_0 + \alpha_x q_x^2 + \alpha_y q_y^2 - \alpha_z q_z^2 \quad , \quad \alpha_{x,y,z} > 0.$$

b) Show that for ω close to ω_0 , the (derivative of) the density of states is of the form

$$n'(\omega) = \begin{cases} \text{const.} & : \ \omega > \omega_0 \\ c(\omega_0 - \omega)^{-1/2} & : \ \omega < \omega_0 \end{cases}$$

(6 points)

Exercise 3: Density of states of the hypercubic lattice

Consider a *d*-dimensional dispersion of the form

$$\varepsilon(\vec{k}) = -\sum_{i=1}^{d} \cos k_i$$
, with $k_i \in [-\pi, \pi]$.

The corresponding density of states is given by

$$N_d(\varepsilon) = \frac{1}{(2\pi)^d} \int \mathrm{d}^d k \, \delta(\varepsilon - \varepsilon(\vec{k})) \; .$$

- a) Calculate the density of states for the one-dimensional case. (2 points)
- b) Show that for $d \ge 0$, the following recursion relation holds:

$$N_{d+1}(\varepsilon) = \frac{1}{(2\pi)} \int_{-\pi}^{\pi} \mathrm{d}k \, N_d(\varepsilon + \cos k) \; .$$

(2 points)