Solid State Theory

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Sheet 4: return on: Monday, Nov 26, 2012, 12:00 (SR THP)

Exercise 1: Discrete Fourier transformation

Consider a finite lattice L_f with periodic boundary conditions as defined in Sec. 3.3. Let $f(\vec{R}_{\vec{n}})$ be a function defined on the lattice points $\vec{R}_{\vec{n}}$ of L_f. The discrete Fourier transform of f is defined as

$$\bar{f}(\vec{q}_{\vec{m}}) = \sum_{\vec{n}} f(\vec{R}_{\vec{n}}) e^{-i\vec{q}_{\vec{m}}\cdot\vec{R}_{\vec{n}}} \ ,$$

with $\sum_{\vec{n}}$ the sum over all $\vec{R}_{\vec{n}}$ of L_f. Due to the periodic boundary conditions, the allowed $\vec{q}$-values are given by

$$\vec{q}_{\vec{m}} = \sum_{\beta=1}^{d} \frac{m_\beta}{N_\beta}\vec{b}_\beta \quad , \quad m_\beta = 0, 1, \ldots, N_\beta - 1 \ .$$

Show that

$$\frac{1}{N}\sum_{\vec{m}} e^{i\vec{q}_{\vec{m}}\cdot(\vec{R}_{\vec{i}}-\vec{R}_{\vec{j}})} = \delta_{\vec{R}_{\vec{i}},\vec{R}_{\vec{j}}} \ ,$$

where $N := \prod_{\beta=1}^{d} N_\beta$ is the total number of sites in L_f. Using the above identity, show that the inverse Fourier transform is given by

$$f(\vec{R}_{\vec{n}}) = \frac{1}{N}\sum_{\vec{m}} \bar{f}(\vec{q}_{\vec{m}}) e^{i\vec{q}_{\vec{m}}\cdot\vec{R}_{\vec{n}}} \ .$$

(4 points)

Exercise 2: Boundary conditions

Consider a one-dimensional Bravais lattice L, with atoms of mass m at lattice vectors $R_n = na$, $n \in \mathbb{Z}$, and an effective potential of the form

$$V_\mathrm{eff} = \alpha \sum_n (u_{n+1} - u_n)^2 \ .$$

A finite version of this lattice consists of lattice vectors $R_n = na$ with $n = 0, 1, \ldots, N-1$.

a) Determine the dynamical matrix for the case of periodic boundary conditions. (1 point)

b) Calculate the spectrum of ω-values $\{\omega_j\}$. (3 points)

c) Consider now the case of fixed boundary conditions. What is the proper finite form of the effective potential for this case? Determine the dynamical matrix. (1 point)

d) Calculate – with a suitable ansatz – the eigenvalues of the dynamical matrix and compare the result with b). (3 points)

Exercise 3: Einstein model

In the Einstein model, we assume that the frequencies $\omega_l(\vec{q})$ are given by

$$\omega_l(\vec{q}) = \omega_0 \ , \ \text{for all } l, \vec{q} \ .$$

a) Calculate the energy E of the ionic system under this assumption. (2 points)

b) Give the exact expression for the specific heat C_V and discuss this quantity in the limit of high and low temperature. (2 points)

Exercise 4: Thermodynamics of a 1d lattice

Consider again the one-dimensional model of Exercise 2. For periodic boundary conditions we arrive at a dispersion relation for the phonons which can be written as

$$\omega(q_n) = \sqrt{\frac{8\alpha}{m}} \sin\left(\frac{q_n a}{2}\right) \quad , \quad \text{with} \ \ q_n = \frac{n}{N}\frac{2\pi}{a} \quad , \quad n = 0, 1, \ldots, N-1 \ .$$

a) Calculate the energy E and the specific heat C_V in the limit of high temperature T. (2 points)

b) Show that in the limit $N \to \infty$ (thermodynamic limit) the energy E can be written as

$$E = \frac{Na}{\pi} \int_0^{\pi/a} \mathrm{d}q \, \hbar\omega(q) \left(\frac{1}{\exp(\beta\hbar\omega(q)) - 1} + \frac{1}{2} \right)$$

(2 points)